

Validation Document Criteria Form

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Procedure: 19-1 Revision: 4 Page 1 of 1

1. Software Name: FMT
2. Software Version ID (proposed): 2.40 2.4 8/21/98
3. Document Version ID: 2.4
4. WPO #: 51587
5. Is the following information included, as applicable?

(a) computer program and version tested	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R
(b) computer hardware and operating system used	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R
(c) test equipment and calibrations, where applicable	<input type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R
(d) date of test	<input type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R
(e) tester	<input type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R
(f) simulation models used, where applicable	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R
(g) test problem input and output files	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input checked="" type="checkbox"/> N/R
(h) results and acceptability	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R
(i) action taken in connection with any deviations noted	<input type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R
(j) person evaluating the tests	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R
6. Test Result Validation
The test results were compared to the following (check one or more):

- hand calculations,	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R
- manual inspection,	<input type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R
- calculations using comparable proven problems,	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R
- empirical data and information from confirmed published data and correlations and/or technical literature,	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R
- other validated software of similar purpose,	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	<input type="checkbox"/> N/A	<input type="checkbox"/> N/R
- other independent software of similar purpose.	<input type="checkbox"/> Yes	<input type="checkbox"/> No	<input checked="" type="checkbox"/> N/A	<input type="checkbox"/> N/R
7. Test Documentation Acceptability
Do the tests meet the acceptance criteria identified in an approved VVP? Yes No N/A N/R
8. Test Documentation Repeatability
Are the tests documented in sufficient detail such that they can be repeated? Yes No N/A N/R
9. Computer File Documentation
Are the test case input and output files included in the Validation Document? Yes No N/A N/R
10. Understandability of Documentation
Are the validation methods, test data, results, and conclusions documented in a form that can be understood by an independent, technically competent individual? Yes No N/A N/R

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**WIPP PA
VALIDATION DOCUMENT**

for

FMT (Version 2.40)

Document Version 2.4

WPO# 51587

October 19, 1998

Information Only

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1.0 INTRODUCTION

The purpose of this document is to summarize the results of the testing activities prescribed in the RD/VVP for Version 2.40 of FMT and to provide evaluations based on those results. The FMT code has previously undergone a complete WIPP QAP 19-1 quality assurance process.

1.1 Software Identifier

FMT version 2.40 (WIPP PA Code Prefix: FMT)

1.2 Points of Contact

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2.0 TESTING ENVIRONMENT

Testing for FMT was performed in the following computer environment:

Hardware platform: DEC Alpha
Operating System: OpenVMS version 7.1
Directory: WP\$NONPA_TESTROOT:[FMT]

3.0 TEST TOOLS

The testing tools which were used as part of the software validation are described in **Table 3.0.1**.

Table 3.0.1 Software Testing Tools

Tool Name	Usage
FORTRAN-Lint (FLINT)	Source Code Analyzer used to identify non ANSI standard coding.
DECset SCA	Source Code analyzer used to identify uncalled modules, to display the calling tree, and to identify the modules used in the analysis.
DECset PCA	Performance Coverage Analyzer, used to identify any unexercised modules
DEC FORTRAN Compiler version EV6.2-508-274	Compiler, used to create the executables and identify compilation errors and warnings.

4.0 STATIC ANALYSIS

For FMT, static analysis was performed using both the source code analyzer FLINT and the source code analyzer DECset-SCA . The analysis was performed in the directory of

WP\$NONPA_TESTROOT:[FMT.SCA]

FLINT was used to detect non-ANSI standard FORTRAN coding. DECset-SCA was used to reveal any uncalled modules, to display the calling tree, and to identify the modules used in the analysis.

4.1 FLINT Analysis: Procedure and Results

PROCEDURE: Since FMT is a multimodule program, FLINT was used on a file created by appending all the modules together. The resulting file is FMT_QB0204.FOR. The file resulting from running FLINT,

FMT_FLINT_QB0204.FLI,

is shown in **Figure 4.1.1**.

RESULTS: As a result of running FLINT, it was noted that several variables were defined but not referenced. This was as expected by the code sponsor.

Figure 4.1.1 FLINT Output for Code Modules

```
FORTRAN-lint    Rev 4.12                      19-Oct-98  10:15:41  Page 1
Default options: /WARNINGS /USAGE /SUPPRESS=207,276,76,261 /NOTREE /NOXREF
Command options: /OUTPUT=fmt_qb0204.fli

>>> Source analysis:

Directory WP$NONPA_TESTROOT:[000000.FMT.FLINT.TEMP]

FMT_QB0204.FOR;1

*****
      Program FMT                               File FMT_QB0204.FOR       Line 1873
FMT_QB0204.FOR:FMT line 2377:
USAGE WARNING #127- local variable CDUM3 is set but never referenced.

FMT_QB0204.FOR:FMT line 2358:
USAGE WARNING #127- local variable TEMP is set but never referenced.

*****
      Subroutine FRACSET                         File FMT_QB0204.FOR       Line 2427
FMT_QB0204.FOR:FRACSET line 2496:
USAGE WARNING #127- local variable ITEMP is set but never referenced.

FMT_QB0204.FOR:FRACSET line 2478:
USAGE WARNING #127- local variable TEMP is set but never referenced.

FMT_QB0204.FOR:FRACSET line 2479:
USAGE WARNING #127- local variable DUMMY1 is set but never referenced.

FMT_QB0204.FOR:FRACSET line 2496:
USAGE WARNING #127- local variable DUMMY2 is set but never referenced.

*****
```

4.2 SCA Analysis: Procedure and Results

PROCEDURE: DECset-SCA was invoked during the build process. The build process was performed using the build script WP_BUILD.COM developed by the SCMS librarian. The build script was fetched from the WP library with the following commands:

```
libwp
cfe wp_build.com
```

The build script is self-contained and is executed in the directory containing the needed input files with the command,

```
@wp_build
```

During the build process, the input file, the input file FMT.MMS is required and is fetched from SCMS. That input file is shown in **Figure 4.2.1**.

As a result of the build process, a debug executable capable of doing PCA analysis was created and the SCA code analyzer created the three output files. These files are listed in **Table 4.2.1** along with a brief description of each file and a reference to where a listing of each file can be found in this document.

Table 4.2.1 Files Created by the SCA Code Analyzer

Output File	Description	Figure
FMT_SCA_MOD_NOT_REF.TXT	A listing of the modules in the code that are not referenced	Figure 4.2.1
FMT_CALLTREE.TXT	A listing of the calling tree for the code	Figure 4.2.2
SCA\$EVENT.DAT	A binary file containing information about the SCA process	

Following the build process, SCA was invoked at the VMS \$ prompt and the following commands were executed on the SCA\$EVENT.DAT file in the WP\$NONPA_TESTROOT: [FMT.SCA] directory:

```
SCA> set lib []
SCA> show module/all/output=FMT_modules_QB0204.out
SCA> exit
```

This procedure converts information in the binary file to ASCII format. The resulting ASCII file, FMT_MODULES_QB0204.OUT, is shown in **Figure 4.2.3**.

The somewhat generic text filenames were changed to include the version number for unique identification prior to submitting them into SCMS. That is,

```
FMT_SCA_MOD_NOT_REF.TXT became FMT_SCA_MOD_NOT_REF_QB0204.TXT and
FMT_CALLTREE.TXT became FMT_CALLTREE_QB0204.TXT.
```

RESULTS: The SCA procedure revealed that the main program itself was not called, as was expected. In addition, the following function ITOCHAR was uncalled. Examination of the call tree output showed that the function was called, and when the DEC search utility was used on the FMT_QB0204.FOR source file, it was clearly shown that in fact the function ITOCHAR was called several times. The anomaly of the finding by SCA cannot be explained, but it is believed that there are no uncalled subroutines or functions in FMT. The file resulting from using the DEC search utility, FMT_ITOCHAR_QB0204.SEA is shown in **Figure 4.2.4**.

Figure 4.2.1 SCA Output File of Modules Not Referenced

FMT procedure	
FMT\1	SUBROUTINE or PROGRAM declaration
ITOCHAR function	
ITOCHAR\1	FUNCTION declaration

Figure 4.2.2 SCA Call Tree Output
(Page 1 of 2)

```
ABS function
DISABLE routine
EHSETUP routine calls
. INT function
FRACSET routine
ONEFLSH routine calls
. ABS function (See above)
. ABUCALC routine
. BATCH routine calls
. . ABUCALC routine (See above)
. . BATCHPR routine calls
. . . ACTBDOT routine calls
. . . . DLOG function
. . . . DSQRT function
. . . DENSITY function
. . . DEXP function
. . . DLOG10 function
. . CANONIC routine calls
. . . DABS function
. . CHKEQUI routine calls
. . . DEXP function (See above)
. . . DLOG function (See above)
. . . SORT routine
. . DETECT routine calls
. . . ABUCALC routine (See above)
. . . DABS function (See above)
. . . DSQRT function (See above)
. . DLOG function (See above)
. . DLOG10 function (See above)
. . EHCALC routine calls
. . . DLOG function (See above)
. . . INT function (See above)
. . EQUILIB routine calls
. . . DABS function (See above)
. . . FORCER routine
. . . HESDIAG routine
. . . MAKENUV routine calls
. . . . CANONIC routine (See above)
. . . . OPTIMIZE routine calls
. . . . . LININDP function calls
. . . . . DSQRT function (See above)
. . . . SHFTCTL routine calls
. . . . . SHFTPRD routine
. . . . . SHFTRID routine
. . . . . SORT routine (See above)
. . . MOLCALC routine calls
. . . . INITGES routine calls
. . . . . ABUCALC routine (See above)
. . . . . CANONIC routine (See above)
. . . . . FEASBL routine calls
. . . . . LPROG routine calls
. . . . . . ABS function (See above)
. . . . . . PVT routine
. . . . . OPTIMIZE routine (See above)
. . . . . SORT routine (See above)
. . . . MAKENUV routine (See above)
. . . MUCALC routine calls
. . . . ACTBDOT routine (See above)
. . . APITZER routine calls
. . . . BCALC routine calls
. . . . . DEXP function (See above)
. . . . . EXP function
. . . . . GPITZ function
. . . . . GPMPITZ function
. . . . . INT function (See above)
. . . . . DABS function (See above)
```

Figure 4.2.2 SCA Call Tree Output
(Page 2 of 2)

```
. . . . . DLOG function (See above)
. . . . . DSQRT function (See above)
. . . . . PSICALC routine calls
. . . . .   CTHETA routine calls
. . . . .   JPITZER routine calls
. . . . .   DEXP function (See above)
. . . . . DABS function (See above)
. . . . . DLOG function (See above)
. . . SWITCH routine
. . IDXELEM routine calls
. . . SORT routine (See above)
. . INITGES routine (See above)
. . OPTIMIZE routine (See above)
. . RIDOABU routine calls
. . . DABS function (See above)
. . SORT routine (See above)
. . VSFCHG routine calls
. . . DABS function (See above)
. . . IDXELEM routine (See above)
. . . INITGES routine (See above)
. . . RIDOABU routine (See above)
. DABS function (See above)
. EHSETUP routine (See above)
. PRTINIT routine calls
. . INT function (See above)
PREFLOW routine calls
. FLASHIJ routine calls
. . ABUCALC routine (See above)
. . BATCH routine (See above)
. . DABS function (See above)
. SDOMAIN routine calls
. . MOLETOC routine calls
. . . DENSITY function (See above)
PRTINIT routine (See above)
READDAT routine calls
. RDPITZR routine calls
. . DSQRT function (See above)
. . INT function (See above)
SETFCO2 routine calls
. DFLOAT function
. DLOG function (See above)
. INT function (See above)
. ITOCHAR variable
. LOG10 function
SETPH routine calls
. DLOG function (See above)
. INT function (See above)
. ITOCHAR variable (See above)
TITRATE routine calls
. ABUCALC routine (See above)
BATCH routine (See above)
DFLOAT function (See above)
. EXP function (See above)
. LOG function
. TITRPT routine calls
. . LOG10 function (See above)
```

Figure 4.2.3 SCA Output File of All Modules Included in Static Analysis

Module	#	Ident	Language	Compiled	
ABUCALC	1	01	FORTRAN	25-Sep-1998 13:46	
ACTBDOT	1	01	FORTRAN	25-Sep-1998 13:46	
APITZER	1	01	FORTRAN	25-Sep-1998 13:46	
BATCH	1	01	FORTRAN	25-Sep-1998 13:46	
BATCHPR	1	01	FORTRAN	25-Sep-1998 13:46	
BCALC	1	01	FORTRAN	25-Sep-1998 13:46	Old ANA format
CANONIC	1	01	FORTRAN	25-Sep-1998 13:46	
CHKEQUI	1	01	FORTRAN	25-Sep-1998 13:46	
CTHETA	1	01	FORTRAN	25-Sep-1998 13:46	
DENSITY	1	01	FORTRAN	25-Sep-1998 13:46	
DETECT	1	01	FORTRAN	25-Sep-1998 13:46	
DISABLE	1	01	FORTRAN	25-Sep-1998 13:46	
EHCALC	1	01	FORTRAN	25-Sep-1998 13:46	
EHSETUP	1	01	FORTRAN	25-Sep-1998 13:46	
EQUILIB	1	01	FORTRAN	25-Sep-1998 13:46	
FEASBL	1	01	FORTRAN	25-Sep-1998 13:46	
FLASHIJ	1	01	FORTRAN	25-Sep-1998 13:46	
FMT	1	01	FORTRAN	25-Sep-1998 13:46	
FORCER	1	01	FORTRAN	25-Sep-1998 13:46	
FRACSET	1	01	FORTRAN	25-Sep-1998 13:47	
HESDIAG	1	01	FORTRAN	25-Sep-1998 13:47	
IDXELEM	1	01	FORTRAN	25-Sep-1998 13:47	
INITGES	1	01	FORTRAN	25-Sep-1998 13:47	
ITOCHAR	1	01	FORTRAN	25-Sep-1998 13:47	
JPITZER	1	01	FORTRAN	25-Sep-1998 13:47	
LININDP	1	01	FORTRAN	25-Sep-1998 13:47	
LPROG	1	01	FORTRAN	25-Sep-1998 13:47	
MAKENUV	1	01	FORTRAN	25-Sep-1998 13:47	
MOLCALC	1	01	FORTRAN	25-Sep-1998 13:47	
MOLETOC	1	01	FORTRAN	25-Sep-1998 13:47	
MUCALC	1	01	FORTRAN	25-Sep-1998 13:47	
ONEFLSH	1	01	FORTRAN	25-Sep-1998 13:47	
OPTIMIZE	1	01	FORTRAN	25-Sep-1998 13:47	
PREFLOW	1	01	FORTRAN	25-Sep-1998 13:47	
PRTINIT	1	01	FORTRAN	25-Sep-1998 13:47	
PSICALC	1	01	FORTRAN	25-Sep-1998 13:47	
PVT	1	01	FORTRAN	25-Sep-1998 13:47	
RDPITZR	1	01	FORTRAN	25-Sep-1998 13:47	
READDAT	1	01	FORTRAN	25-Sep-1998 13:47	
RIDOABU	1	01	FORTRAN	25-Sep-1998 13:47	
SDOMAIN	1	01	FORTRAN	25-Sep-1998 13:47	
SETFCO2	1	01	FORTRAN	25-Sep-1998 13:47	
SETPH	1	01	FORTRAN	25-Sep-1998 13:47	
SHFTCTL	1	01	FORTRAN	25-Sep-1998 13:47	
SHFTPRD	1	01	FORTRAN	25-Sep-1998 13:47	
SHFTRID	1	01	FORTRAN	25-Sep-1998 13:47	
SORT	1	01	FORTRAN	25-Sep-1998 13:47	
SWITCH	1	01	FORTRAN	25-Sep-1998 13:47	
TITRATE	1	01	FORTRAN	25-Sep-1998 13:47	
TITRPRT	1	01	FORTRAN	25-Sep-1998 13:47	
VSECHG	1	01	FORTRAN	25-Sep-1998 13:47	

Figure 4.2.4 Search Utility Output File, FMT_ITOCHAR.SEA

```
CHARACTER FUNCTION ITOCHAR(DIGIT)
  WRITE(06,*) 'ITOCHAR RECIEVED THE VALUE ',DIGIT
  WRITE(06,*) 'VALUE PASSED TO ITOCHAR MUST BE BETWEEN 0 AND 9'
  STOP 'BAD VALUE PASSED TO ITOCHAR()'
  ITOCHAR='0'
  ITOCHAR='1'
  ITOCHAR='2'
  ITOCHAR='3'
  ITOCHAR='4'
  ITOCHAR='5'
  ITOCHAR='6'
  ITOCHAR='7'
  ITOCHAR='8'
  ITOCHAR='9'
C CMS REPLACEMENT HISTORY, Element FMT_ITOCHAR.FOR
C CMS REPLACEMENT HISTORY, Element FMT_ITOCHAR.FOR
CHARACTER ITOCHAR
EXTERNAL ITOCHAR
  STR(1:1)=ITOCHAR(DIGIT)
  STR(11:11)=ITOCHAR(DIGIT)
  STR(9:9)=ITOCHAR(DIGIT)
  STR(10:10)=ITOCHAR(DIGIT)
CHARACTER ITOCHAR
EXTERNAL ITOCHAR
  STR(2:2)=ITOCHAR(DIGIT)
  STR(11:11)=ITOCHAR(DIGIT)
```

5.0 COVERAGE ANALYSIS

The coverage analysis for FMT was performed using DECset PCA. A unique executable, called FMT_TEST_PCA_QB0204.EXE was created for the purpose of coverage analysis. This executable was generated by using the SCMS build script, WP_BUILD.COM and placed in the WP\$NONPA_TESTROOT:[FMT.EXE] directory. The coverage analysis was performed in the WP\$NONPA_TESTROOT:[FMT.PCA] directory.

The command file FMT_PCA_QB0204.COM, shown in **Figure 5.0.1**, was used to run the FMT test cases with PCA. A log of the PCA analysis, FMT_PCA_QB0204.LOG, resulting from running the script was created. An edited listing of that file can be seen in **Figure 5.0.2**. It was edited to remove echo from the running of the code. The unedited log file has been retained in SCMS. The cumulative PCA results, FMT_COVER_CUM_QB0204.TXT, for all the test cases can be seen in **Figure 5.0.3**.

Modules ACTBDOT, EHCALC, and VSFCHG perform the functionalities that are not supported by the current version of the code, and therefore they are not covered in the coverage analysis. Module SHFTRID is used to eliminate one of the species involved in a solids-only reaction in the numerical iteration for chemical equilibrium calculations. The module is called only occasionally, depending on testing problems. Therefore, the zero coverage of module SHFTRID for the given set of testing cases is not unexpected. All the other modules are covered in the coverage analysis.

Figure 5.0.1 Script Used to Run Test Cases for PCA Analysis
(Page 1 of 6)

```
C
$ set noon
$!
$!*****
$! This file does PCA coverage analysis on FMT
$!*****
$!
$ define/nolog lib$debug sys$library:pca$collector.exe
$ TESTDIR_SYM == "WP$NONPA_TESTROOT:[FMT.PCA]
$ FMT == "$ WP$NONPA_TESTROOT:[FMT.EXE]FMT_TEST_PCA_QB0204.EXE"
$ define /proc testdir wp$nonpa_testroot:[fmt.pca]
$ sh sym testdir_sym
$ IF F$MODE () .EQS. "BATCH" .AND. F$ENVIRONMENT ("DEPTH") .EQ. 0 THEN -
    SET DEFAULT 'TESTDIR_SYM'
$!
$! If the cum pca file exists, rename it so we get a new file
$ rename fmt_pca_cum_qb0204.pca *.pca_old
$!
$ libfmt
$!
$!*****
$! Define initial databases
$!
$ CFG FMT_PH_970407.CHEMDAT QB0204
$ define chemdat fmt_ph_970407.chemdat
$ CFG FMT_HMW_AM3PU3TH4NP5_960823.RHOMIN QB0204
$ define rhomin fmt_hmw_am3pu3th4np5_960823.rhomin
$!*****
$! TEST CASE #1
$!
$ write sys$output " STARTING TEST CASE #1"
$!
$ CFE FMT_SPC_BM.IN
$! CFG FMT_SPC_BM.IN QB0204
$ define input fmt_spc_bm.in
$ CFG FMT_SPC_BM.INGUESS QB0204
$ define inguess fmt_spc_bm.inguess
$!
$ define output fmt_spc_bm_pca_QB0204.out
$ define for088 fmt_spc_bm_pca_QB0204.for088
$!
$ FMT
    set data/append fmt_pca_cum_qb0204.pca
    set cover program by routine
    go
$!
$ del fmt_spc_bm_pca_qb0204.out;*
$ del fmt_spc_bm_pca_qb0204.for088;*
$ del fmt_spc_bm.in;*
$ del fmt_spc_bm.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #1"
$ write sys$output " "
$!*****
$! TEST CASE #2
$!
$ write sys$output " STARTING TEST CASE #2"
$!
$ CFE FMT_NP_NACL_BM.IN
$! CFG FMT_NP_NACL_BM.IN QB0204

$ define input fmt_np_nacl_bm.in
$ CFG FMT_NP_NACL_BM.INGUESS QB0204
$ define inguess fmt_np_nacl_bm.inguess
$!
$ define output fmt_np_nacl_bm_pca_qb0204.out
$ define titrate fmt_np_nacl_bm_pca_qb0204.titrate
$ define moles fmt_np_nacl_bm_pca_qb0204.moles
```

Figure 5.0.1 Script Used to Run Test Cases for PCA Analysis
(Page 2 of 6)

```
$!  
$ FMT  
    set data/append fmt_pca_cum_qb0204.pca  
    set cover program by routine  
    go  
$!  
$ del fmt_np_nacl_bm_pca_qb0204.out;*  
$ del fmt_np_nacl_bm_pca_qb0204.titrate;*  
$ del fmt_np_nacl_bm.in;*  
$ del fmt_np_nacl_bm.inguess;*  
$!  
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #2"  
$ write sys$output " "  
$!*****  
$! TEST CASE #3  
$!  
$ write sys$output " STARTING TEST CASE #3"  
$!  
$ CFE FMT_THO2_6MNACL.IN  
$! CFG FMT_THO2_6MNACL.IN QB0204  
$ define input fmt_tho2_6mnacl.in  
$ CFG FMT_THO2_6MNACL.INGUESS QB0204  
$ define inguess fmt_tho2_6mnacl.inguess  
$!  
$ define output fmt_tho2_6mnacl_pca_qb0204.out  
$ define titrate fmt_tho2_6mnacl_pca_qb0204.titrate  
$ define moles fmt_tho2_6mnacl_pca_qb0204.moles  
$!  
$ FMT  
    set data/append fmt_pca_cum_qb0204.pca  
    set cover program by routine  
    go  
$!  
$ del fmt_tho2_6mnacl_pca_qb0204.out;*  
$ del fmt_tho2_6mnacl_pca_qb0204.titrate;*  
$ del fmt_tho2_6mnacl.in;*  
$ del fmt_tho2_6mnacl.inguess;*  
$!  
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #3"  
$ write sys$output " "  
$!*****  
$! TEST CASE #4 - PART 1  
$!  
$ write sys$output " STARTING TEST CASE #4"  
$ write sys$output " PART 1"  
$!  
$ CFG FMT_AM_NA2CO3.IN QB0204  
$ define input fmt_am_na2co3.in  
$ CFG FMT_AM_NA2CO3.INGUESS QB0204  
$ define inguess fmt_am_na2co3.inguess  
$!  
$ define output fmt_am_na2co3_pca_qb0204.out  
$ define titrate fmt_am_na2co3_pca_qb0204.titrate  
$!  
$ FMT  
    set data/append fmt_pca_cum_qb0204.pca  
    set cover program by routine  
    go  
$!  
$ del fmt_am_na2co3_pca_qb0204.out;*  
$ del fmt_am_na2co3_pca_qb0204.titrate;*  
$ del fmt_am_na2co3.in;*  
$ del fmt_am_na2co3.inguess;*  
$!  
$!*****  
$! TEST CASE #4 - PART 2  
$!
```

Figure 5.0.1 Script Used to Run Test Cases for PCA Analysis
(Page 3 of 6)

```
$ write sys$output " PART 2"
$!
$ CFG FMT_AM_NAHCO3.IN QB0204
$ define input fmt_am_nahco3.in
$ CFG FMT_AM_NAHCO3.INGUESS QB0204
$ define inguess fmt_am_nahco3.inguess
$!
$ define output fmt_am_nahco3_pca_qb0204.out
$ define titrate fmt_am_nahco3_pca_qb0204.titrate
$ define moles fmt_am_nahco3_pca_qb0204.moles
$!
$ FMT
    set data/append fmt_pca_cum_qb0204.pca
    set cover program by routine
    go
$!
$ del fmt_am_nahco3_pca_qb0204.out;*
$ del fmt_am_nahco3_pca_qb0204.titrate;*
$ del fmt_am_nahco3.in;*
$ del fmt_am_nahco3.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #4"
$ write sys$output " "
$!*****
$! TEST CASE #5 - PART 1
$!
$ write sys$output " STARTING TEST CASE #5"
$ write sys$output " PART 1"
$!
$ CFG FMT_AMPO4_SO4_BM1.IN QB0204
$ define input fmt_ampo4_so4_bm1.in
$ CFG FMT_AMPO4_SO4_BM1.INGUESS QB0204
$ define inguess fmt_ampo4_so4_bm1.inguess
$!
$ define output fmt_ampo4_so4_bm1_pca_qb0204.out
$ define titrate fmt_ampo4_so4_bm1_pca_qb0204.titrate
$ define moles fmt_ampo4_so4_bm1_pca_qb0204.moles
$!
$ FMT
    set data/append fmt_pca_cum_qb0204.pca
    set cover program by routine
    go
$!
$ del fmt_ampo4_so4_bm1_pca_qb0204.out;*
$ del fmt_ampo4_so4_bm1_pca_qb0204.titrate;*
$ del fmt_ampo4_so4_bm1.in;*

$ del fmt_ampo4_so4_bm1.inguess;*
$!
$!*****
$! TEST CASE #5 - PART 1
$!
$ write sys$output " PART 2"
$!
$ CFG FMT_AMPO4_SO4_BM2.IN QB0204
$ define input fmt_ampo4_so4_bm2.in
$ CFG FMT_AMPO4_SO4_BM2.INGUESS QB0204
$ define inguess fmt_ampo4_so4_bm2.inguess
$!
$ define output fmt_ampo4_so4_bm2_pca_qb0204.out
$ define titrate fmt_ampo4_so4_bm2_pca_qb0204.titrate
$ define moles fmt_ampo4_so4_bm2_pca_qb0204.moles
$!
$ FMT
    set data/append fmt_pca_cum_qb0204.pca
    set cover program by routine
    go
$!
```

Figure 5.0.1 Script Used to Run Test Cases for PCA Analysis
(Page 4 of 6)

```
$ del fmt_ampo4_so4_bm2_pca_qb0204.out;*
$ del fmt_ampo4_so4_bm2_pca_qb0204.titrate;*
$ del fmt_ampo4_so4_bm2.in;*
$ del fmt_ampo4_so4_bm2.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #5"
$ write sys$output " "
$!*****
$! TEST CASE #6
$!
$ write sys$output " STARTING TEST CASE #6"
$!
$ CFG FMT_FCO2_PH_FIXED.IN QB0204
$ define input fmt_fco2_ph_fixed.in
$ CFG FMT_FCO2_PH_FIXED.INGUESS
$! CFG FMT_FCO2_PH_FIXED.INGUESS QB0204
$ define inguess fmt_fco2_ph_fixed.inguess
$!
$ define output fmt_fco2_ph_fixed_pca_qb0204.out
$ define titrate fmt_fco2_ph_fixed_pca_qb0204.titrate
$ define moles fmt_fco2_ph_fixed_pca_qb0204.moles
$!
$ FMT
  set data/append fmt_pca_cum_qb0204.pca
  set cover program by routine
  go
$!
$ del fmt_fco2_ph_fixed_pca_qb0204.out;*
$ del fmt_fco2_ph_fixed.in;*
$ del fmt_fco2_ph_fixed.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #6"
$ write sys$output " "
$!*****
$! TEST CASE #7 - PART 1
$!
$ write sys$output " STARTING TEST CASE #7"
$ write sys$output " PART 1"
$!

$ CFG FMT_INVAR_M.IN QB0204
$ define input fmt_invar_m.in
$ CFG FMT_INVAR_M.INGUESS QB0204
$ define inguess fmt_invar_m.inguess
$!
$ define output fmt_invar_m_pca_qb0204.out
$ define titrate fmt_invar_m_pca_qb0204.titrate
$ define moles fmt_invar_m_pca_qb0204.moles
$!
$ FMT
  set data/append fmt_pca_cum_qb0204.pca
  set cover program by routine
  go
$!
$ del fmt_invar_m_pca_qb0204.out;*
$ del fmt_invar_m.in;*
$ del fmt_invar_m.inguess;*
$!
$!*****
$! TEST CASE #7 - PART 2
$!
$ write sys$output " PART 2"
$!
$ CFG FMT_INVAR_B3.IN QB0204
$ define input fmt_invar_b3.in
$ CFG FMT_INVAR_B3.INGUESS QB0204
$ define inguess fmt_invar_b3.inguess
$!
```

Figure 5.0.1 Script Used to Run Test Cases for PCA Analysis
(Page 5 of 6)

```
$ define output fmt_invar_b3_pca_qb0204.out
$ define titrate fmt_invar_b3_pca_qb0204.titrate
$ define moles fmt_invar_b3_pca_qb0204.moles
$!
$ FMT
  set data/append fmt_pca_cum_qb0204.pca
  set cover program by routine
  go
$!
$ del fmt_invar_b3_pca_qb0204.out;*
$ del fmt_invar_b3.in;*
$ del fmt_invar_b3.inguess;*
$!
$!*****
$! TEST CASE #7 - PART 3
$!
$ write sys$output " PART 3"
$!
$ CFG FMT_INVAR_K4.IN QB0204
$ define input fmt_invar_k4.in
$ CFG FMT_INVAR_K4.INGUESS QB0204
$ define inguess fmt_invar_k4.inguess
$!
$ define output fmt_invar_k4_pca_qb0204.out
$ define titrate fmt_invar_k4_pca_qb0204.titrate
$ define moles fmt_invar_k4_pca_qb0204.moles
$!
$ FMT
  set data/append fmt_pca_cum_qb0204.pca
  set cover program by routine
  go
$!

$ del fmt_invar_k4_pca_qb0204.out;*
$ del fmt_invar_k4.in;*
$ del fmt_invar_k4.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #7"
$ write sys$output " "
$!*****
$! TEST CASE #8
$!
$ write sys$output " STARTING TEST CASE #8"
$!
$ CFG FMT_AMTHNP_SPC.IN QB0204
$ define input fmt_amthnp_spc.in
$ CFG FMT_AMTHNP_SPC.INGUESS QB0204
$ define inguess fmt_amthnp_spc.inguess
$!
$ define output fmt_amthnp_spc_pca_qb0204.out
$ define titrate fmt_amthnp_spc_pca_qb0204.titrate
$ define moles fmt_amthnp_spc_pca_qb0204.moles
$!
$ FMT
  set data/append fmt_pca_cum_qb0204.pca
  set cover program by routine
  go
$!
$ del fmt_amthnp_spc_pca_qb0204.out;*
$ del fmt_amthnp_spc.in;*
$ del fmt_amthnp_spc.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #8"
$ write sys$output " "
$!*****
$! run the PCA analyzer on the collected data
$!
```

Figure 5.0.1 Script Used to Run Test Cases for PCA Analysis
(Page 6 of 6)

```
$ write sys$output " STARTING THE CUMULATIVE PCA"  
$!  
$ PCA fmt_pca_cum_qb0204.pca  
  tab /cover program by routine  
  file fmt_cover_cum_qb0204.txt  
  exit  
$!  
$ write sys$output -  
  " SUCCESSFUL COMPLETION OF PCA FOR TEST CASES 1 THROUGH 8"  
$!*****  
$ DEL FMT_*.CHEMDAT;*  
$ DEL FMT_*.RHOMIN;*  
$!*****
```

Figure 5.0.2 Edited Listing of the Log File of the PCA Coverage Analysis
(Page 1 of 5)

```
%DCL-I-SUPERSEDE, previous value of TESTDIR has been superseded
  TESTDIR_SYM == "WP$NONPA_TESTROOT:[FMT.PCA]"
%RENAME-E-SEARCHFAIL, error searching for
WP$NONPA TESTROOT:[000000.FMT.PCA]FMT_PCA_CUM_QB0204.PCA;
-RMS-E-FNF, file not found
%CMS-I-LIBIS, library is WP$NONPA_CMSROOT:[FMT]
%CMS-S-LIBSET, library set
-CMS-I-SUPERSEDE, library list superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_PH_970407.CHEMDAT fetched
%DCL-I-SUPERSEDE, previous value of CHEMDAT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 2 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_AM3PU3TH4NP5_960823.RHOMIN
fetched
%DCL-I-SUPERSEDE, previous value of RHOMIN has been superseded
STARTING TEST CASE #1
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_SPC_BM.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_SPC_BM.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of FOR088 has been superseded

  PCA Collector Version V4.5-4

%PCA-I-CREFILE, creating file FMT_PCA_CUM_QB0204.PCA
%PCA-I-BEGINCOL, data collection begins
SINGLE BATCH EQUILIBRATION COMPLETED
%PCA-I-ENDCOL, data collection ends
  SUCCESSFUL COMPLETION OF TEST CASE #1

STARTING TEST CASE #2
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_NP_NACL_BM.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_NP_NACL_BM.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded

  PCA Collector Version V4.5-4

%PCA-I-BEGINCOL, data collection begins
End of AutoTitration Problem
%PCA-I-ENDCOL, data collection ends
  SUCCESSFUL COMPLETION OF TEST CASE #2

STARTING TEST CASE #3
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]
```


Figure 5.0.2 Edited Listing of the Log File of the PCA Coverage Analysis
(Page 2 of 5)

```
%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_THO2_6MNAACL.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_THO2_6MNAACL.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded

  PCA Collector Version V4.5-4

%PCA-I-BEGINCOL, data collection begins
End of AutoTitration Problem
%PCA-I-ENDCOL, data collection ends
  SUCCESSFUL COMPLETION OF TEST CASE #3

  STARTING TEST CASE #4
  PART 1
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AM_NA2CO3.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AM_NA2CO3.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded

  PCA Collector Version V4.5-4

%PCA-I-BEGINCOL, data collection begins
End of AutoTitration Problem
%PCA-I-ENDCOL, data collection ends
  PART 2
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AM_NAHC03.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AM_NAHC03.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded

  PCA Collector Version V4.5-4

%PCA-I-BEGINCOL, data collection begins
End of AutoTitration Problem
%PCA-I-ENDCOL, data collection ends
  SUCCESSFUL COMPLETION OF TEST CASE #4

  STARTING TEST CASE #5
  PART 1
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMPO4_SO4_BM1.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
```

Figure 5.0.2 Edited Listing of the Log File of the PCA Coverage Analysis
(Page 3 of 5)

```
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMPO4_SO4_BM1.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded

  PCA Collector Version V4.5-4

%PCA-I-BEGINCOL, data collection begins
End of AutoTitration Problem
%PCA-I-ENDCOL, data collection ends
  PART 2
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMPO4_SO4_BM2.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMPO4_SO4_BM2.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded

  PCA Collector Version V4.5-4

%PCA-I-BEGINCOL, data collection begins
End of AutoTitration Problem
%PCA-I-ENDCOL, data collection ends

SUCCESSFUL COMPLETION OF TEST CASE #5

  STARTING TEST CASE #6
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_FC02_PH_FIXED.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_FC02_PH_FIXED.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded

  PCA Collector Version V4.5-4

%PCA-I-BEGINCOL, data collection begins
SINGLE BATCH EQUILIBRATION COMPLETED
%PCA-I-ENDCOL, data collection ends
  SUCCESSFUL COMPLETION OF TEST CASE #6

  STARTING TEST CASE #7
  PART 1
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_M.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]
```

Figure 5.0.2 Edited Listing of the Log File of the PCA Coverage Analysis
(Page 4 of 5)

```
%CMS-S-FETCHED, generation 2 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_M.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
```

PCA Collector Version V4.5-4

```
%PCA-I-BEGINCOL, data collection begins
SINGLE BATCH EQUILIBRATION COMPLETED
%PCA-I-ENDCOL, data collection ends
PART 2
Your CMS library list consists of:
WP$NONPA_CMSROOT:[FMT]
```

```
%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_B3.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
WP$NONPA_CMSROOT:[FMT]
```

```
%CMS-S-FETCHED, generation 2 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_B3.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
```

PCA Collector Version V4.5-4

```
%PCA-I-BEGINCOL, data collection begins
SINGLE BATCH EQUILIBRATION COMPLETED
%PCA-I-ENDCOL, data collection ends
PART 3
Your CMS library list consists of:
WP$NONPA_CMSROOT:[FMT]
```

```
%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_K4.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
WP$NONPA_CMSROOT:[FMT]
```

```
%CMS-S-FETCHED, generation 2 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_K4.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
```

PCA Collector Version V4.5-4

```
%PCA-I-BEGINCOL, data collection begins
SINGLE BATCH EQUILIBRATION COMPLETED
%PCA-I-ENDCOL, data collection ends
SUCCESSFUL COMPLETION OF TEST CASE #7
```

```
STARTING TEST CASE #8
Your CMS library list consists of:
WP$NONPA_CMSROOT:[FMT]
```

```
%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMTHNP_SPC.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
WP$NONPA_CMSROOT:[FMT]
```

```
%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMTHNP_SPC.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
```

Figure 5.0.2 Edited Listing of the Log File of the PCA Coverage Analysis
(Page 5 of 5)

%DCL-I-SUPERSEDE, previous value of MOLES has been superseded

PCA Collector Version V4.5-4

%PCA-I-BEGINCOL, data collection begins
SINGLE BATCH EQUILIBRATION COMPLETED
%PCA-I-ENDCOL, data collection ends
SUCCESSFUL COMPLETION OF TEST CASE #8

STARTING THE CUMULATIVE PCA

DEC Performance and Coverage Analyzer Version V4.5-4

DEC Performance and Coverage Analyzer Page 1

Test Coverage Data (507 data points total) - "*"

Bucket Name	Data Count	Percent
ABUCALC\ ABUCALC	12	2.4%
APITZER\ APITZER	12	2.4%
BATCH\ BATCH	12	2.4%
BATCHPR\ BATCHPR	12	2.4%
BCALC\ BCALC	12	2.4%
BCALC\BCALC\ GPITZ	12	2.4%
GMPITZ	12	2.4%
CANONIC\ CANONIC	12	2.4%
CHKEQUI\ CHKEQUI	12	2.4%

%PCA-I-CREFILE, creating file WPSNONPA_TESTROOT:[000000.FMT.PCA]FMT_COVER_CUM_QB0204.TXT;1
SUCCESSFUL COMPLETION OF PCA FOR TEST CASES 1 THROUGH 8

Figure 5.0.3 Cumulative Results of the PCA Coverage Analysis
 (Page 1 of 3)

DEC Performance and Coverage Analyzer

Page 1

Test Coverage Data (507 data points total) - "**"

Bucket Name	Data Count	Percent
ABUCALC\ ABUCALC	12	2.4%
APITZER\ APITZER	12	2.4%
BATCH\ BATCH	12	2.4%
BATCHPR\ BATCHPR	12	2.4%
BCALC\ BCALC	12	2.4%
BCALC\BCALC\ GPITZ	12	2.4%
GPMPITZ	12	2.4%
CANONIC\ CANONIC	12	2.4%
CHKEQUI\ CHKEQUI	12	2.4%
CTHETA\ CTHETA	12	2.4%
DENSITY\ DENSITY	12	2.4%
DETECT\ DETECT	12	2.4%
DISABLE\ DISABLE	12	2.4%
EQUILIB\ EQUILIB	12	2.4%
FMT\ FMT	12	2.4%
FORCER\ FORCER	12	2.4%
HESDIAG\ HESDIAG	12	2.4%
IDXELEM\ IDXELEM	12	2.4%
JPITZER\ JPITZER	12	2.4%
LININDP\ LININDP	12	2.4%
MAKENUV\ MAKENUV	12	2.4%
MOLCALC\ MOLCALC	12	2.4%
MUCALC\ MUCALC	12	2.4%
OPTIMIZE\ OPTIMIZE	12	2.4%
PRTINIT\ PRTINIT	12	2.4%
PSICALC\ PSICALC	12	2.4%

DEC Performance and Coverage Analyzer

Page 2

Test Coverage Data (507 data points total) - "**"

Bucket Name	Data Count	Percent
RDPIITZR\ RDPIITZR	12	2.4%
READDAT\ READDAT	12	2.4%

Figure 5.0.3 Cumulative Results of the PCA Coverage Analysis
 (Page 2 of 3)

RIDOABU\ RIDOABU	12	2.4%
SETFCO2\ SETFCO2	12	2.4%
SETPH\ SETPH	12	2.4%
SHFTCTL\ SHFTCTL	12	2.4%
SHFTPRD\ SHFTPRD	12	2.4%
SORT\ SORT	12	2.4%
SWITCH\ SWITCH	12	2.4%
FEASBL\ FEASBL	8	1.6%
INITGES\ INITGES	8	1.6%
LPROG\ LPROG	8	1.6%
PVT\ PVT	8	1.6%
EHSETUP\ EHSETUP	6	1.2%
FLASHIJ\ FLASHIJ	6	1.2%
FRACSET\ FRACSET	6	1.2%
MOLETOC\ MOLETOC	6	1.2%
ONEFLSH\ ONEFLSH	6	1.2%
PREFLOW\ PREFLOW	6	1.2%
SDOMAIN\ SDOMAIN	6	1.2%
TITRATE\ TITRATE	6	1.2%
TITRPRT\ TITRPRT	6	1.2%
ITOCHAR\ ITOCHAR	1	0.2%
ACTBDOT\ ACTBDOT	0	0.0%
EHCALC\ EHCALC	0	0.0%
SHFTRID\ SHFTRID	0	0.0%

DEC Performance and Coverage Analyzer

Page 3

Test Coverage Data (507 data points total) - ""

Bucket Name	Data Count	Percent
SYSTEM\$SERVICE\ SYSTEM\$SERVICE	0	-
SYSTEM\$SPACE\ SYSTEM\$SPACE	0	-
VSFCHG\ VSFCHG	0	0.0%

DEC Performance and Coverage Analyzer

Page 4

Test Coverage Data (507 data points total) - ""

PCA Version V4.5-4 6-OCT-1998 14:29:37

Figure 5.0.3 Cumulative Results of the PCA Coverage Analysis
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```
TABULATE Command Summary Information:
Number of buckets tallied:                55

Test Coverage Data - "*"
Number of covered buckets:                49    89.1%
Number of acceptably not covered buckets:  0     0.0%
Number of remaining not covered buckets:   4     7.3%
Number of buckets with no coverage data:   2     3.6%

Data count in largest defined bucket:      12     2.4%
Data count in all defined buckets:         507   100.0%
Data count not in defined buckets:         0     0.0%
Portion of above count in P0 space:        0     0.0%
Number of PC values in P1 space:           0     0.0%
Number of PC values in system space:       0     0.0%

Total number of data values collected:     507   100.0%

Command qualifiers and parameters used:
Qualifiers:
  /COVERAGE /DESCENDING /NOMINIMUM /NOMAXIMUM
  /NOCUMULATIVE /NOSOURCE /ZEROS /NOSCALE /NOCREATOR_PC
  /NOPATHNAME /NOCHAIN_NAME /NOWRAP /NOPARENT_TASK /NOKEEP /NOTREE
  /FILL=("*", "0", "x", "@", ":", "#", "/", "+")
  /NOSTACK_DEPTH /NOMAIN_IMAGE
Node specifications:
  PROGRAM_ADDRESS BY ROUTINE

No filters are defined
```

6.0 FUNCTIONAL TESTING

A total of 8 test cases were provided for FMT functional testing. The test cases were run in the directory WP\$NONPA_TESTROOT:[FMT.TESTCASES], and all files associated with the functional testing are located in this directory. To run the test cases a script, FMT_TEST_QB0204.COM, was used. A listing of the script can be seen in **Figure 6.0.1**. A log of the testing procedure, FMT_TEST_QB0204.LOG, was created during the running of the script. A listing of that log file can be seen in **Figure 6.0.2**

All required input files were fetched using the CFG command from the CMS procedures. Two databases are required for all test cases. They are

FMT_PH_070407.CHEMDAT, and
FMT_HMW_AM3PU3TH4NP5_960823.RHOMIN

A list of the functional requirements for FMT follows. A summary of the requirements tested by each of the eight test cases can be found in **Table 6.0.1**. An evaluation of the individual test cases can be found in Sections 6.1-6.8.

Functional Requirements

- R.1 - FMT predicts mineral solubilities in the Na-K-Mg-Ca-H-Cl-SO₄-OH-HCO₃-CO₃-CO₂-B(OH)₃-H₂O to high ionic strength at 25°.
- R.2 - FMT predicts solubility behaviour of Am(III), Th(IV), and Np(V) in brines such as those found in Castile, Rustler, and Salado Formations near the Waste Isolation Pilot Plant (WIPP).
- R.3 - The batch simulation mode, also know as flash problems, calculates chemical equilibrium for a given set of element abundance.
- R.4 - FMT supports three titration calculation modes: user-specified increments, linear increments, and logarithmic increments.
- R.5 - FMT fixes solution pH or f_{CO_2} as specified in an input file.
- R.6 - FMT disables any chemical species as specified in an input file.

Performance Requirements

This code has no performance requirements.

Attribute Requirements

This code has no attribute requirements.

External Interface Requirements

- R.7 - The parameters in the actinide series used in the FMT database are calculated by NONLIN or other equivalent means.

Other Requirements

There are no other requirements for FMT that need verification.

Table 6.0.1 Requirement Coverage by Test Cases

Requirement Type	Requirement Number	Test Cases							
		1	2	3	4	5	6	7	8
Functional	R.1	X						X	
	R.2		X	X	X	X			X
	R.3	X						X	X
	R.4		X	X	X	X			
	R.5						X		
	R.6						X		
External Interface	R.7		X	X	X	X			X

Figure 6.0.1 Script Used for Running Test Cases for Functional Analysis
(Page 1 of 5)

```
$ set noon
$!
$!*****
$! This file does TEST coverage analysis on FMT
$!*****
$!
$ define/nolog lib$debug sys$library:TEST$collector.exe
$ TESTDIR_SYM == "WP$NONPA TESTROOT:[FMT.TESTCASES]
$ FMT == "$ WP$NONPA_PRODRÖÖT:[FMT.EXE]FMT_QB0204.EXE"
$ define /proc testdir wp$nonpa_testroot:[FMT.TESTCASES]
$ sh sym testdir_sym
$ IF F$MODE () .EQS. "BATCH" .AND. F$ENVIRONMENT ("DEPTH") .EQ. 0 THEN -
    SET DEFAULT 'TESTDIR_SYM'
$!
$ libfmt
$!
$!*****
$! Define initial databases
$!
$ CFG FMT_PH_970407.CHEMDAT QB0204
$ define chemdat fmt_ph_970407.chemdat
$ CFG FMT_HMW_AM3PU3TH4NP5_960823.RHOMIN QB0204
$ define rhomin fmt_hmw_am3pu3th4np5_960823.rhomin
$!*****
$! TEST CASE #1
$!
$ write sys$output " STARTING TEST CASE #1"
$!
$ CFE FMT_SPC_BM.IN
$! CFG FMT_SPC_BM.IN QB0204
$ define input fmt_spc_bm.in
$ CFG FMT_SPC_BM.INGUESS QB0204
$ define inguess fmt_spc_bm.inguess
$!
$ define output fmt_spc_bm_QB0204.out
$ define for088 fmt_spc_bm_QB0204.for088
$!
$ FMT
$!
$ CFG FMT_SPC_BM_230.OUT PA97
$ CFG FMT_SPC_BM_230.FOR088 PA97
$!
$ DIFF/OUTPUT=FMT_SPC_BM_OUT.DIF -
    FMT_SPC_BM_QB0204.OUT -
    FMT_SPC_BM_230.OUT
$ DIFF/OUTPUT=FMT_SPC_BM_FOR088.DIF -
    FMT_SPC_BM_QB0204.FOR088 -
    FMT_SPC_BM_230.FOR088
$!
$ del fmt_spc_bm.in;*
$ del fmt_spc_bm.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #1"
$ write sys$output " "
$!*****
$! TEST CASE #2
$!
$ write sys$output " STARTING TEST CASE #2"
$!
$ CFE FMT_NP_NACL_BM.IN
$! CFG FMT_NP_NACL_BM.IN QB0204
$ define input fmt_np_nacl_bm.in
$ CFG FMT_NP_NACL_BM.INGUESS QB0204
$ define inguess fmt_np_nacl_bm.inguess
$!
$ define output fmt_np_nacl_bm_qb0204.out
$ define titrate fmt_np_nacl_bm_qb0204.titrate
$ define moles fmt_np_nacl_bm_qb0204.moles
```

Figure 6.0.1 Script Used for Running Test Cases for Functional Analysis
(Page 2 of 5)

```
$!  
$ FMT  
$!  
$ del fmt_np_nacl_bm.in;*  
$ del fmt_np_nacl_bm.inguess;*  
$!  
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #2"  
$ write sys$output " "  
$!*****  
$! TEST CASE #3  
$!  
$ write sys$output " STARTING TEST CASE #3"  
$!  
$ CFG FMT_THO2_6MNACL.IN  
$! CFG FMT_THO2_6MNACL.IN QB0204  
$ define input fmt_tho2_6mnacl.in  
$ CFG FMT_THO2_6MNACL.INGUESS QB0204  
$ define inguess fmt_tho2_6mnacl.inguess  
$!  
$ define output fmt_tho2_6mnacl_qb0204.out  
$ define titrate fmt_tho2_6mnacl_qb0204.titrate  
$ define moles fmt_tho2_6mnacl_qb0204.moles  
$!  
$ FMT  
$!  
$ del fmt_tho2_6mnacl.in;*  
$ del fmt_tho2_6mnacl.inguess;*  
$!  
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #3"  
$ write sys$output " "  
$!*****  
$! TEST CASE #4 - PART 1  
$!  
$ write sys$output " STARTING TEST CASE #4"  
$ write sys$output " PART 1"  
$!  
$ CFG FMT_AM_NA2CO3.IN QB0204  
$ define input fmt_am_na2co3.in  
$ CFG FMT_AM_NA2CO3.INGUESS QB0204  
$ define inguess fmt_am_na2co3.inguess  
$!  
$ define output fmt_am_na2co3_qb0204.out  
$ define titrate fmt_am_na2co3_qb0204.titrate  
$!  
$ FMT  
$!  
$ del fmt_am_na2co3.in;*  
$ del fmt_am_na2co3.inguess;*  
$!  
$!*****  
$! TEST CASE #4 - PART 2  
$!  
$ write sys$output " PART 2"  
$!  
$ CFG FMT_AM_NAHC03.IN QB0204  
$ define input fmt_am_nahco3.in  
$ CFG FMT_AM_NAHC03.INGUESS QB0204  
$ define inguess fmt_am_nahco3.inguess  
$!  
$ define output fmt_am_nahco3_qb0204.out  
$ define titrate fmt_am_nahco3_qb0204.titrate  
$ define moles fmt_am_nahco3_qb0204.moles  
$!  
$ FMT  
$!  
$ del fmt_am_nahco3.in;*  
$ del fmt_am_nahco3.inguess;*  
$!
```

Figure 6.0.1 Script Used for Running Test Cases for Functional Analysis
(Page 3 of 5)

```
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #4"
$ write sys$output " "
$!*****
$! TEST CASE #5 - PART 1
$!
$ write sys$output " STARTING TEST CASE #5"
$ write sys$output " PART 1"
$!
$ CFG FMT_AMPO4_SO4_BM1.IN QB0204
$ define input fmt_ampo4_so4_bml.in
$ CFG FMT_AMPO4_SO4_BM1.INGUESS QB0204
$ define inguess fmt_ampo4_so4_bml.inguess
$!
$ define output fmt_ampo4_so4_bml_qb0204.out
$ define titrate fmt_ampo4_so4_bml_qb0204.titrate
$ define moles fmt_ampo4_so4_bml_qb0204.moles
$!
$ FMT
$!
$ del fmt_ampo4_so4_bml.in;*
$ del fmt_ampo4_so4_bml.inguess;*
$!
$!*****
$! TEST CASE #5 - PART 1
$!
$ write sys$output " PART 2"
$!
$ CFG FMT_AMPO4_SO4_BM2.IN QB0204
$ define input fmt_ampo4_so4_bm2.in
$ CFG FMT_AMPO4_SO4_BM2.INGUESS QB0204
$ define inguess fmt_ampo4_so4_bm2.inguess
$!
$ define output fmt_ampo4_so4_bm2_qb0204.out
$ define titrate fmt_ampo4_so4_bm2_qb0204.titrate
$ define moles fmt_ampo4_so4_bm2_qb0204.moles
$!
$ FMT
$!
$ del fmt_ampo4_so4_bm2.in;*
$ del fmt_ampo4_so4_bm2.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #5"
$ write sys$output " "
$!*****
$! TEST CASE #6
$!
$ write sys$output " STARTING TEST CASE #6"
$!
$ CFG FMT_FCO2_PH_FIXED.IN QB0204
$ define input fmt_fco2_ph_fixed.in
$ CFG FMT_FCO2_PH_FIXED.INGUESS QB0204
$ define inguess fmt_fco2_ph_fixed.inguess
$!
$ define output fmt_fco2_ph_fixed_qb0204.out
$ define titrate fmt_fco2_ph_fixed_qb0204.titrate
$ define moles fmt_fco2_ph_fixed_qb0204.moles
$!
$ FMT
$!
$ del fmt_fco2_ph_fixed.in;*
$ del fmt_fco2_ph_fixed.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #6"
$ write sys$output " "
$!*****
$! TEST CASE #7 - PART 1
$!
```

Figure 6.0.1 Script Used for Running Test Cases for Functional Analysis
(Page 4 of 5)

```
$ write sys$output " STARTING TEST CASE #7"
$ write sys$output " PART 1"
$!
$ CFG FMT_INVAR_M.IN QB0204
$ define input fmt_invar_m.in
$ CFG FMT_INVAR_M.INGUESS QB0204
$ define inguess fmt_invar_m.inguess
$!
$ define output fmt_invar_m_qb0204.out
$ define titrate fmt_invar_m_qb0204.titrate
$ define moles fmt_invar_m_qb0204.moles
$!
$ FMT
$!
$ del fmt_invar_m.in;*
$ del fmt_invar_m.inguess;*
$!
$! *****
$! TEST CASE #7 - PART 2
$!
$ write sys$output " PART 2"
$!
$ CFG FMT_INVAR_B3.IN QB0204
$ define input fmt_invar_b3.in
$ CFG FMT_INVAR_B3.INGUESS QB0204
$ define inguess fmt_invar_b3.inguess
$!
$ define output fmt_invar_b3_qb0204.out
$ define titrate fmt_invar_b3_qb0204.titrate
$ define moles fmt_invar_b3_qb0204.moles
$!
$ FMT
$!
$ del fmt_invar_b3.in;*
$ del fmt_invar_b3.inguess;*
$!
$! *****
$! TEST CASE #7 - PART 3
$!
$ write sys$output " PART 3"
$!
$ CFG FMT_INVAR_K4.IN QB0204
$ define input fmt_invar_k4.in
$ CFG FMT_INVAR_K4.INGUESS QB0204
$ define inguess fmt_invar_k4.inguess
$!
$ define output fmt_invar_k4_qb0204.out
$ define titrate fmt_invar_k4_qb0204.titrate
$ define moles fmt_invar_k4_qb0204.moles
$!
$ FMT
$!
$ del fmt_invar_k4.in;*
$ del .fmt_invar_k4.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #7"
$ write sys$output " "
$! *****
$! TEST CASE #8
$!
$ write sys$output " STARTING TEST CASE #8"
$!
$ CFG FMT_AMTHNP_SPC.IN QB0204
$ define input fmt_amthnp_spc.in
$ CFE FMT_AMTHNP_SPC.INGUESS
$! CFG FMT_AMTHNP_SPC.INGUESS QB0204
$ define inguess fmt_amthnp_spc.inguess
$!
```

Figure 6.0.1 Script Used for Running Test Cases for Functional Analysis
(Page 5 of 5)

```
$ define output fmt_amthnp_spc_qb0204.out
$ define titrate fmt_amthnp_spc_qb0204.titrate
$ define moles fmt_amthnp_spc_qb0204.moles
$!
$ FMT
$!
$ del fmt_amthnp_spc.in;*
$ del fmt_amthnp_spc.inguess;*
$!
$ write sys$output " SUCCESSFUL COMPLETION OF TEST CASE #8"
$ write sys$output " "
$!*****
!
$ write sys$output -
" SUCCESSFUL COMPLETION OF TEST CASES 1 THROUGH 8"
$!*****
$ DEL FMT *.CHEMDAT;*
$ DEL FMT *.RHOMIN;*
$!*****
```

Figure 6.0.2 Edited Listing of the Functional Testing Log File
(Page 1 of 3)

```
%DCL-I-SUPERSEDE, previous value of TESTDIR has been superseded
  TESTDIR SYM == "WP$NONPA TESTROOT:[FMT.TESTCASES]"
%CMS-I-LIBIS, library is WP$NONPA_CMSROOT:[FMT]
%CMS-S-LIBSET, library set
-CMS-I-SUPERSEDE, library list superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_PH_970407.CHEMDAT fetched
%DCL-I-SUPERSEDE, previous value of CHEMDAT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 2 of element WP$NONPA_CMSROOT:[FMT]FMT_HMW_AM3PU3TH4NP5_960823.RHOMIN fetched
%DCL-I-SUPERSEDE, previous value of RHOMIN has been superseded
STARTING TEST CASE #1
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_SPC_BM.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_SPC_BM.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUSS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of FOR088 has been superseded
SINGLE BATCH EQUILIBRATION COMPLETED
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_SPC_BM_230.OUT fetched
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_SPC_BM_230.FOR088 fetched
SUCCESSFUL COMPLETION OF TEST CASE #1

STARTING TEST CASE #2
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_NP_NACL_BM.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_NP_NACL_BM.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUSS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
End of AutoTitration Problem
SUCCESSFUL COMPLETION OF TEST CASE #2

STARTING TEST CASE #3
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_THO2_6MNAACL.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_THO2_6MNAACL.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUSS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
End of AutoTitration Problem
SUCCESSFUL COMPLETION OF TEST CASE #3

STARTING TEST CASE #4
PART 1
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]
```

Figure 6.02 Edited Listing of the Functional Testing Log File
(Page 2 of 3)

```
%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AM_NA2CO3.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AM_NA2CO3.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGRESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
End of AutoTitration Problem
PART 2
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AM_NAHC03.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AM_NAHC03.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGRESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
End of AutoTitration Problem
SUCCESSFUL COMPLETION OF TEST CASE #4

STARTING TEST CASE #5
PART 1
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMPO4_SO4_BM1.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMPO4_SO4_BM1.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGRESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
End of AutoTitration Problem
PART 2
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMPO4_SO4_BM2.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMPO4_SO4_BM2.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGRESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
End of AutoTitration Problem
SUCCESSFUL COMPLETION OF TEST CASE #5

STARTING TEST CASE #6
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_FCO2_PH_FIXED.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded

Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_FCO2_PH_FIXED.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGRESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded

SINGLE BATCH EQUILIBRATION COMPLETED
SUCCESSFUL COMPLETION OF TEST CASE #6
```


Figure 6.0.2 Edited Listing of the Functional Testing Log File
(Page 3 of 3)

```
STARTING TEST CASE #7
PART 1
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_M.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 2 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_M.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
SINGLE BATCH EQUILIBRATION COMPLETED
PART 2
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_B3.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 2 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_B3.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
SINGLE BATCH EQUILIBRATION COMPLETED
PART 3
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_K4.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 2 of element WP$NONPA_CMSROOT:[FMT]FMT_INVAR_K4.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
SINGLE BATCH EQUILIBRATION COMPLETED
SUCCESSFUL COMPLETION OF TEST CASE #7

STARTING TEST CASE #8
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMTHNP_SPC.IN fetched
%DCL-I-SUPERSEDE, previous value of INPUT has been superseded
Your CMS library list consists of:
  WP$NONPA_CMSROOT:[FMT]

%CMS-S-FETCHED, generation 1 of element WP$NONPA_CMSROOT:[FMT]FMT_AMTHNP_SPC.INGUESS fetched
%DCL-I-SUPERSEDE, previous value of INGUESS has been superseded
%DCL-I-SUPERSEDE, previous value of OUTPUT has been superseded
%DCL-I-SUPERSEDE, previous value of TITRATE has been superseded
%DCL-I-SUPERSEDE, previous value of MOLES has been superseded
SINGLE BATCH EQUILIBRATION COMPLETED
SUCCESSFUL COMPLETION OF TEST CASE #8

SUCCESSFUL COMPLETION OF TEST CASES 1 THROUGH 8
```

6.1 Test Case #1: Speciation in WIPP SPC (Salado Primary Constituent) Brine

6.1.1 Test Objectives

The "batch" mode is used to calculate the species concentrations in the WIPP SPC brine. The SPC brine has been used to represent the WIPP Salado brine in various experiments measuring colloidal and dissolved actinide concentrations. This test case is to test the FMT equilibrium calculation for nonradioactive chemical components. It will test functional requirements R.1 and R.3.

6.1.2 Test Procedures

This test case was run using the script FMT_TEST_QB0204.COM. This command file is shown in **Figure 6.0.2**.

6.1.3 Input/Output Files

The following is a list of all files associated with Test Case #1:

Command file:

FMT_TEST_QB0204.COM

Input files:

FMT_SPC_BM.IN

(See **Figure 6.1.1**)

FMT_SPC_BM.INGUESS

Output files:

FMT_SPC_BM_QB0204.OUT

(See **Figure 6.1.2**)

In this case, FMT_SPC_BM.INGUESS is used as a dummy input file and thus it is not listed here.

Figure 6.1.1 Listing of the Input File FMT_SPC_BM.IN

```
'Benchmark BATCH Problem:  SPC Brine, Appx.B SAND91-2111'  
'CHEMFILE'  
'BATCH' 'UNUSED'  
'DISABLE_SPECIES' 0  
'nSET_FC02' 0.0  
'nSET_PH' 0.0  
  
'nMOLES' 'nEXACT'  
1.11084063E+02 Hydrogen  
5.57650233E+01 Oxygen  
2.00000000E+00 Sodium  
8.40000000E-01 Potassium  
1.55999951E+00 Magnesium  
1.64000000E-02 Calcium  
5.83000000E+00 Chlorine  
4.36000000E-02 Sulfur  
5.07101504E-03 Carbon  
0.00000000E+00 PosIon:EL  
5.32000000E-02 NegIon:EL  
0.00000000E+00 Oxalate:EL  
2.18000000E-02 Boron  
1.09000000E-02 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
2.71310752E-15 Charge:EL
```

Figure 6.1.2 Edited Listing of the Output File FMT_SPC_BM_QB0204.OUT

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Molarity	mg/liter
H2O	WATER	8.42589E-01	4.96550E+01	8.94545E+05
Cl-	Cl-	5.83002E+00	5.21521E+00	1.84895E+05
Na+	Na+	2.00001E+00	1.78909E+00	4.11309E+04
Mg++	Mg++	1.55395E+00	1.39008E+00	3.37858E+04
K+	K+	8.40002E-01	7.51420E-01	2.93792E+04
NegIon	NEGATIVE. ION	5.32001E-02	4.75899E-02	0.00000E+00
SO4=	SO4=	4.36001E-02	3.90022E-02	3.74646E+03
B(OH)3(aq)	B(OH)3(aq)	2.02511E-02	1.81155E-02	1.12012E+03
Ca++	Ca++	1.63816E-02	1.46541E-02	5.87335E+02
Br-	Br-	1.09000E-02	9.75056E-03	7.79109E+02
MgCO3	Magnesite	4.89468E-03	4.37851E-03	3.69171E+02
MgB(OH)4+	MgB(OH)4+	1.12935E-03	1.01026E-03	1.04202E+02
B(OH)4-	B(OH)4-	3.62398E-04	3.24182E-04	2.55582E+01
HCO3-	HCO3-	1.40358E-04	1.25556E-04	7.66107E+00
CO2(aq)	CO2(aq)	2.18481E-05	1.95441E-05	8.60133E-01
CaB(OH)4+	CaB(OH)4+	1.83288E-05	1.63959E-05	1.94979E+00
MgOH+	MgOH+	1.78189E-05	1.59398E-05	6.58509E-01
B3O3(OH)4-	B3O3(OH)4-	1.24753E-05	1.11597E-05	1.65674E+00
MgCO3(aq)	MgCO3(aq)	1.24349E-05	1.11236E-05	9.37879E-01
CO3=	CO3=	1.58972E-06	1.42208E-06	8.53379E-02
B4O5(OH)4=	B4O5(OH)4=	3.54373E-07	3.17003E-07	6.06319E-02
CaCO3(aq)	CaCO3(aq)	1.18621E-07	1.06112E-07	1.06207E-02
H+	H+	1.02365E-07	9.15701E-08	9.22935E-05
OH-	OH-	8.80709E-08	7.87833E-08	1.33989E-03
HSO4-	HSO4-	2.20433E-08	1.97187E-08	1.91401E-03

6.1.4 Evaluation

Since no modification has been made for the component Na-K-Ca-Mg-Cl-C-S-B-Br-H-O in FMT_PH_970407.CHEMDAT, the calculated species concentrations were expected to agree with those calculated by FMT version 2.3. The agreement was expected to be to 6 significant digits.

Figure 6.1.3 shows an edited listing of the output file FMT_SPC_BM_230.OUT resulting from calculations from version 2.3 of FMT. The entire output file is stored in SCMS. Tables 6.1.1 and 6.1.2 show the comparisons between the concentration calculated by versions 2.3 and 2.4 of FMT

Figure 6.1.3 Edited Listing of the Output File FMT_SPC_BM_230.OUT

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Molarity	mg/liter
H2O	WATER	8.42589E-01	4.96550E+01	8.94545E+05
Cl-	Cl-	5.83002E+00	5.21521E+00	1.84895E+05
Na+	Na+	2.00001E+00	1.78909E+00	4.11309E+04
Mg++	Mg++	1.55395E+00	1.39008E+00	3.37858E+04
K+	K+	8.40002E-01	7.51420E-01	2.93792E+04
NegIon.....	NEGATIVE.ION	5.32001E-02	4.75899E-02	0.00000E+00
SO4=	SO4=	4.36001E-02	3.90022E-02	3.74646E+03
B(OH)3(aq)	B(OH)3(aq)	2.02511E-02	1.81155E-02	1.12012E+03
Ca++	Ca++	1.63816E-02	1.46541E-02	5.87335E+02
Br-	Br-	1.09000E-02	9.75056E-03	7.79109E+02
MgCO3	Magnesite	4.89468E-03	4.37851E-03	3.69171E+02
MgB(OH)4+	MgB(OH)4+	1.12935E-03	1.01026E-03	1.04202E+02
B(OH)4-	B(OH)4-	3.62399E-04	3.24182E-04	2.55582E+01
HCO3-	HCO3-	1.40358E-04	1.25556E-04	7.66107E+00
CO2(aq)	CO2(aq)	2.18481E-05	1.95441E-05	8.60133E-01
CaB(OH)4+	CaB(OH)4+	1.83288E-05	1.63959E-05	1.94979E+00
MgOH+	MgOH+	1.78189E-05	1.59398E-05	6.58509E-01
B3O3(OH)4-	B3O3(OH)4-	1.24753E-05	1.11597E-05	1.65674E+00
MgCO3(aq)	MgCO3(aq)	1.24349E-05	1.11236E-05	9.37879E-01
CO3=	CO3=	1.58972E-06	1.42208E-06	8.53379E-02
B4O5(OH)4=	B4O5(OH)4=	3.54373E-07	3.17003E-07	6.06319E-02
CaCO3(aq)	CaCO3(aq)	1.18621E-07	1.06112E-07	1.06207E-02
H+	H+	1.02365E-07	9.15701E-08	9.22935E-05
OH-	OH-	8.80709E-08	7.87833E-08	1.33989E-03
HSO4-	HSO4-	2.20433E-08	1.97187E-08	1.91401E-03

**Table 6.1.1 Comparison of Concentrations Calculated with Versions 2.3 and 2.4
 Of FMT (Molality and Molarity)**

	Molality			Molarity		
	Version 2.4	Version 2.3	Difference	Version 2.4	Version 2.3	Difference
H2O	8.42589E-01	8.42589E-01	0.00E+00	4.96550E+01	4.96550E+01	0.00E+00
Cl-	5.83002E+00	5.83002E+00	0.00E+00	5.21521E+00	5.21521E+00	0.00E+00
Na+	2.00001E+00	2.00001E+00	0.00E+00	1.78909E+00	1.78909E+00	0.00E+00
Mg++	1.55395E+00	1.55395E+00	0.00E+00	1.39008E+00	1.39008E+00	0.00E+00
K+	8.40002E-01	8.40002E-01	0.00E+00	7.51420E-01	7.51420E-01	0.00E+00
Neglon	5.32001E-02	5.32001E-02	0.00E+00	4.75899E-02	4.75899E-02	0.00E+00
SO4=	4.36001E-02	4.36001E-02	0.00E+00	3.90022E-02	3.90022E-02	0.00E+00
B(OH)3(aq)	2.02511E-02	2.02511E-02	0.00E+00	1.81155E-02	1.81155E-02	0.00E+00
Ca++	1.63816E-02	1.63816E-02	0.00E+00	1.46541E-02	1.46541E-02	0.00E+00
Br-	1.09000E-02	1.09000E-02	0.00E+00	9.75056E-03	9.75056E-03	0.00E+00
MgCO3	4.89468E-03	4.89468E-03	0.00E+00	4.37851E-03	4.37851E-03	0.00E+00
MgB(OH)4+	1.12935E-03	1.12935E-03	0.00E+00	1.01026E-03	1.01026E-03	0.00E+00
B(OH)4-	3.62398E-04	3.62399E-04	-1.00E-09	3.24182E-04	3.24182E-04	0.00E+00
HCO3-	1.40358E-04	1.40358E-04	0.00E+00	1.25556E-04	1.25556E-04	0.00E+00
CO2(aq)	2.18481E-05	2.18481E-05	0.00E+00	1.95441E-05	1.95441E-05	0.00E+00
CaB(OH)4+	1.83288E-05	1.83288E-05	0.00E+00	1.63959E-05	1.63959E-05	0.00E+00
MgOH+	1.78189E-05	1.78189E-05	0.00E+00	1.59398E-05	1.59398E-05	0.00E+00
B3O3(OH)4-	1.24753E-05	1.24753E-05	0.00E+00	1.11597E-05	1.11597E-05	0.00E+00
MgCO3(aq)	1.24349E-05	1.24349E-05	0.00E+00	1.11236E-05	1.11236E-05	0.00E+00
CO3=	1.58972E-06	1.58972E-06	0.00E+00	1.42208E-06	1.42208E-06	0.00E+00
B4O5(OH)4=	3.54373E-07	3.54373E-07	0.00E+00	3.17003E-07	3.17003E-07	0.00E+00
CaCO3(aq)	1.18621E-07	1.18621E-07	0.00E+00	1.06112E-07	1.06112E-07	0.00E+00
H+	1.02365E-07	1.02365E-07	0.00E+00	9.15701E-08	9.15701E-08	0.00E+00
OH-	8.80709E-08	8.80709E-08	0.00E+00	7.87833E-08	7.87833E-08	0.00E+00
HSO4-	2.20433E-08	2.20433E-08	0.00E+00	1.97187E-08	1.97187E-08	0.00E+00

**Table 6.1.2 Comparison of Concentrations Calculated with Versions 2.3 and 2.4
 Of FMT (mg/liter)**

	mg/liter		
	Version 2.4	Version 2.3	Difference
H2O	8.94545E+05	8.94545E+05	0.00E+00
Cl-	1.84895E+05	1.84895E+05	0.00E+00
Na+	4.11309E+04	4.11309E+04	0.00E+00
Mg++	3.37858E+04	3.37858E+04	0.00E+00
K+	2.93792E+04	2.93792E+04	0.00E+00
Neglon	0.00000E+00	0.00000E+00	0.00E+00
SO4=	3.74646E+03	3.74646E+03	0.00E+00
B(OH)3(aq)	1.12012E+03	1.12012E+03	0.00E+00
Ca++	5.87335E+02	5.87335E+02	0.00E+00
Br-	7.79109E+02	7.79109E+02	0.00E+00
MgCO3	3.69171E+02	3.69171E+02	0.00E+00
MgB(OH)4+	1.04202E+02	1.04202E+02	0.00E+00
B(OH)4-	2.55582E+01	2.55582E+01	0.00E+00
HCO3-	7.66107E+00	7.66107E+00	0.00E+00
CO2(aq)	8.60133E-01	8.60133E-01	0.00E+00
CaB(OH)4+	1.94979E+00	1.94979E+00	0.00E+00
MgOH+	6.58509E-01	6.58509E-01	0.00E+00
B3O3(OH)4-	1.65674E+00	1.65674E+00	0.00E+00
MgCO3(aq)	9.37879E-01	9.37879E-01	0.00E+00
CO3=	8.53379E-02	8.53379E-02	0.00E+00
B4O5(OH)4=	6.06319E-02	6.06319E-02	0.00E+00
CaCO3(aq)	1.06207E-02	1.06207E-02	0.00E+00
H+	9.22935E-05	9.22935E-05	0.00E+00
OH-	1.33989E-03	1.33989E-03	0.00E+00
HSO4-	1.91401E-03	1.91401E-03	0.00E+00

With the exception of the molality of B(OH)4-, all calculated concentrations are identical. For B(OH)4-, the molality calculated by the two versions differed by one in the 6th significant digit. The acceptance criteria is considered to have been met.

6.2 Test Case #2: Solubility of Hydrated $\text{NaNpO}_2\text{CO}_3$ in NaCl Solution

6.2.1 Test Objectives

The “titration” mode of user-specified increments is used to calculate the solubility of hydrated $\text{NaNpO}_2\text{CO}_3$ in a 5.61 molal NaCl solution as a function of carbonate concentration. This test case is to demonstrate the capability of FMT in the prediction of Np behavior in NaCl-dominated solutions. This test case will test functional requirements R.2, R.4, and R.7.

6.2.2 Test Procedures

This test case was run using the script FMT_TEST_QB0204.COM. This command file is shown in **Figure 6.0.2**.

6.2.3 Input/Output Files

The following is a list of all files associated with Test Case #2:

Command file:

FMT_TEST_QB0204.COM

Input files:

FMT_NP_NACL_BM.IN

(See **Figure 6.2.1**)

FMT_NP_NACL_BM.INGUESS

(See **Figure 6.2.2**)

Output files:

FMT_NP_NACL_BM_QB0204.OUT

(See **Figure 6.2.3**)

FMT_NP_NACL_BM_QB0204.TITRATE

(See **Figure 6.2.4**)

Figure 6.2.1 Listing of the Input File FMT_NP_NACL_BM.IN
(Page 1 of 2)

```
'Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl'  
'CHEMFILE'  
  
'TITRATE' 'EXPLICIT'  
'DISABLE_SPECIES' 1  
146  
'nSET_FCO2' 0.0  
'nSET_PH' 0.0  
  
'nMOLES' 'nEXACT'  
1.11017363E+02 Hydrogen  
6.15086815E+01 Oxygen  
5.61000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
1.61000000E+00 Chlorine  
0.00000000E+00 Sulfur  
2.00000001E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
-2.22044605E-15 Charge:EL  
  
'nMOLES' 'nEXACT'  
1.81018363E+02 Hydrogen  
1.40508682E+02 Oxygen  
1.56100000E+01 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
5.61100000E+00 Chlorine  
0.00000000E+00 Sulfur  
1.00000000E+01 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
1.00000000E+01 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
-2.37316632E-15 Charge:EL
```

Figure 6.2.1 Listing of the Input File FMT_NP_NACL_BM.IN
(Page 2 of 2)

```
15 2.25d3 0.0025d0 1.800001d5 'NDXVARIABLE'  
'nDIFFUS',  
'CONVEC',  
'nSSDIFF',  
'nRESTART',  
'nPUSHPULL', 'nMULTINJ',  
  
20 1 20 'nLOTS' 10  
'nTGRAD' 'LINEAR'  
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'  
3  
0.1d0 0.2d0 0.3d0  
1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'  
'nMOLES' 'nEXACT' Plain old pure H2O  
1.11017364E+02 Hydrogen  
5.55086820E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Pu(III)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge  
  
1.d-12 1.d-20 (fracture, matrix permeabilities)  
'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)  
'VAR_AQ_RHO' 1074.9d0  
'nNO X DIFF',  
'UNIFORM',0  
  
'TITRATE', 'ASREAD', 0.1d0, 10.d0, 'nINJSOLIDS'  
0.10000  
0.14251  
0.16  
0.18  
0.20309  
0.22  
0.24  
0.26  
0.28943  
0.41246  
0.58780  
1.1938  
3.4551  
10.000
```

Figure 6.2.2 Listing of the Input File FMT_NP_NACL_BM.INGUESS

(This file is necessary but is intentionally blank for this test case.)

Figure 6.2.3 Edited Listing of the Output File FMT_NP_NACL_BM_QB0204.OUT
(Page 1 of 4)

NPUT file name is:WP\$NONPA TESTROOT:[000000.FMT.TESTCASES]FMT_NP_NACL_BM.IN;1
INGUESS file name is:WP\$NONPA TESTROOT:[000000.FMT.TESTCASES]FMT_NP_NACL_BM.INGUESS;1
OUTPUT file name is:WP\$NONPA TESTROOT:[000000.FMT.TESTCASES]FMT_NP_NACL_BM_QB0204.OUT;1
CHEMDAT file name is:WP\$NONPA TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark TITRATE Problem: Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.4
FMT_ph_970407.chemdat
Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5=== by analogy

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.57464E-01	8.59843E-01	1.003	5.55025E+01	5.00446E+01	9.01564E+05
Na+	Na+	5.61062E+00	3.69881E+00	0.6593	5.61000E+00	5.05833E+00	1.16290E+05
CO3=	CO3=	1.99407E+00	4.09214E-02	2.0522E-02	1.99385E+00	1.79778E+00	1.07884E+05
Cl-	Cl-	1.61018E+00	1.06477E+00	0.6613	1.61000E+00	1.45168E+00	5.14664E+04
HCO3-	HCO3-	6.14734E-03	1.59044E-03	0.2587	6.14666E-03	5.54222E-03	3.38170E+02
OH-	OH-	6.14733E-03	4.86901E-03	0.7921	6.14665E-03	5.54221E-03	9.42580E+01
CO2(aq)	CO2(aq)	2.36876E-09	7.15914E-09	3.022	2.36850E-09	2.13559E-09	9.39868E-05
H+	H+	2.39954E-12	1.77959E-12	0.7416	2.39927E-12	2.16334E-12	2.18043E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31825E-01	7.77969E-01	0.9353	5.55114E+01	4.96916E+01	8.95204E+05
Cl-	Cl-	5.61072E+00	5.29296E+00	0.9434	5.61100E+00	5.02274E+00	1.78071E+05
Na+	Na+	5.61042E+00	5.29216E+00	0.9433	5.61069E+00	5.02247E+00	1.15465E+05
2 [NaNpO2CO3.7/2H2O(s)]		4.99941E+00	1.00000E+00	1.000	4.99965E+00	4.47549E+00	3.71554E+06
NpO2+	NpO2+	6.89566E-04	1.31657E-03	1.909	6.89600E-04	6.17302E-04	1.66083E+02
HCO3-	HCO3-	3.79560E-04	1.40521E-04	0.3702	3.79579E-04	3.39784E-04	2.07326E+01
CO2(aq)	CO2(aq)	3.09916E-04	8.99894E-04	2.904	3.09931E-04	2.77438E-04	1.22100E+01
NpO2CO3-	NpO2CO3-	3.29958E-06	3.96244E-07	0.1201	3.29974E-06	2.95379E-06	9.71964E-01
H+	H+	5.83989E-07	2.29072E-06	3.923	5.84018E-07	5.22790E-07	5.26920E-04
CO3=	CO3=	1.08181E-07	2.80880E-09	2.5964E-02	1.08186E-07	9.68442E-08	5.81154E-03
NpO2OH(aq)	NpO2OH(aq)	1.86099E-08	2.20696E-09	0.1186	1.86108E-08	1.66596E-08	4.76556E-03
OH-	OH-	6.29659E-09	3.42241E-09	0.5435	6.29690E-09	5.63673E-09	9.58656E-05
NpO2(CO3)2==	NpO2(CO3)2==	1.48074E-10	3.06622E-14	2.0707E-04	1.48082E-10	1.32557E-10	5.15732E-05
NpO2(OH)2-	NpO2(OH)2-	2.20062E-14	4.44949E-16	2.0219E-02	2.20073E-14	1.97000E-14	5.97032E-09
NpO2(CO3)3==	NpO2(CO3)3==	1.86478E-15	6.83998E-24	3.6680E-09	1.86487E-15	1.66935E-15	7.49665E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31825E-01	7.77969E-01	0.9353	1.73882E+01	4.96916E+01	8.95204E+05
Cl-	Cl-	5.61072E+00	5.29296E+00	0.9434	1.75757E+00	5.02274E+00	1.78071E+05
Na+	Na+	5.61042E+00	5.29216E+00	0.9433	1.75748E+00	5.02247E+00	1.15465E+05
2 [NaNpO2CO3.7/2H2O(s)]		4.99941E+00	1.00000E+00	1.000	1.56608E+00	4.47549E+00	3.71554E+06
NpO2+	NpO2+	6.89566E-04	1.31657E-03	1.909	2.16008E-04	6.17302E-04	1.66083E+02
HCO3-	HCO3-	3.79560E-04	1.40521E-04	0.3702	1.18898E-04	3.39784E-04	2.07326E+01
CO2(aq)	CO2(aq)	3.09916E-04	8.99894E-04	2.904	9.70819E-05	2.77438E-04	1.22100E+01
NpO2CO3-	NpO2CO3-	3.29958E-06	3.96244E-07	0.1201	1.03360E-06	2.95379E-06	9.71964E-01
H+	H+	5.83989E-07	2.29072E-06	3.923	1.82936E-07	5.22790E-07	5.26920E-04
CO3=	CO3=	1.08181E-07	2.80880E-09	2.5964E-02	3.38880E-08	9.68442E-08	5.81154E-03
NpO2OH(aq)	NpO2OH(aq)	1.86099E-08	2.20696E-09	0.1186	5.82959E-09	1.66596E-08	4.76556E-03
OH-	OH-	6.29659E-09	3.42241E-09	0.5435	1.97242E-09	5.63673E-09	9.58656E-05
NpO2(CO3)2==	NpO2(CO3)2==	1.48074E-10	3.06622E-14	2.0707E-04	4.63846E-11	1.32557E-10	5.15732E-05
NpO2(OH)2-	NpO2(OH)2-	2.20062E-14	4.44949E-16	2.0219E-02	6.89349E-15	1.97000E-14	5.97032E-09
NpO2(CO3)3==	NpO2(CO3)3==	1.86478E-15	6.83998E-24	3.6680E-09	5.84146E-16	1.66935E-15	7.49665E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31846E-01	7.78017E-01	0.9353	1.73927E+01	4.96942E+01	8.95251E+05
Na+	Na+	5.61012E+00	5.29105E+00	0.9431	1.75783E+00	5.02246E+00	1.15465E+05
Cl-	Cl-	5.60975E+00	5.29121E+00	0.9432	1.75772E+00	5.02213E+00	1.78050E+05
2 [NaNpO2CO3.7/2H2O(s)]		4.99837E+00	1.00000E+00	1.000	1.56615E+00	4.47479E+00	3.71497E+06
HCO3-	HCO3-	5.71347E-04	2.11540E-04	0.3702	1.79022E-04	5.11499E-04	3.12102E+01
CO2(aq)	CO2(aq)	2.14053E-04	6.21508E-04	2.904	6.70697E-05	1.91631E-04	8.43364E+00
NpO2+	NpO2+	2.10212E-04	4.01252E-04	1.909	6.58662E-05	1.88192E-04	5.06326E+01
NpO2CO3-	NpO2CO3-	3.29820E-06	3.96241E-07	0.1201	1.03343E-06	2.95271E-06	9.71608E-01
CO3=	CO3=	3.54871E-07	9.21602E-09	2.5970E-02	1.11193E-07	3.17699E-07	1.90649E-02
H+	H+	2.68023E-07	1.05100E-06	3.921	8.39805E-08	2.39948E-07	2.41844E-04
OH-	OH-	1.37231E-08	4.75982E-09	0.5436	4.29988E-09	1.22856E-08	2.08944E-04
NpO2OH(aq)	NpO2OH(aq)	1.23582E-08	1.46611E-09	0.1186	3.87222E-09	1.10637E-08	3.16481E-03
NpO2(CO3)2==	NpO2(CO3)2==	4.85263E-10	1.00606E-13	2.0732E-04	1.52049E-10	4.34432E-10	1.69023E-04
NpO2(OH)2-	NpO2(OH)2-	3.18488E-14	6.44287E-16	2.0230E-02	9.97926E-15	2.85126E-14	8.64109E-09
NpO2(CO3)3==	NpO2(CO3)3==	1.99953E-14	7.36375E-23	3.6827E-09	6.26519E-15	1.79008E-14	8.03881E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31853E-01	7.78036E-01	0.9353	1.73946E+01	4.96950E+01	8.95265E+05
Na+	Na+	5.61003E+00	5.29050E+00	0.9430	1.75800E+00	5.02246E+00	1.15465E+05
Cl-	Cl-	5.60932E+00	5.29056E+00	0.9432	1.75778E+00	5.02183E+00	1.78039E+05
2 [NaNpO2CO3.7/2H2O(s)]		4.99788E+00	1.00000E+00	1.000	1.56617E+00	4.47443E+00	3.71467E+06
HCO3-	HCO3-	7.65975E-04	2.83608E-04	0.3703	2.40032E-04	6.85750E-04	4.18425E+01
CO2(aq)	CO2(aq)	1.16771E-04	3.39044E-04	2.903	3.65923E-05	1.04541E-04	4.60084E+00
NpO2+	NpO2+	6.38093E-05	1.21785E-04	1.909	1.99958E-05	5.71263E-05	1.53696E+01

Figure 6.2.3 Edited Listing of the Output File FMT_NP_NACL_BM_QB0204.OUT
(Page 2 of 4)

NpO2CO3-	NpO2CO3-	3.29766E-06	3.96249E-07	0.1202	1.03338E-06	2.95228E-06	9.71465E-01	-2.96E-13
CO3=	CO3=	1.16916E-06	3.03652E-08	2.5972E-02	3.66376E-07	1.04671E-06	6.28120E-02	-1.36E-08
H+	H+	1.09076E-07	4.27656E-07	3.921	3.41809E-08	9.76521E-08	9.84235E-05	9.67E-09
OH-	OH-	3.37243E-08	1.83335E-08	0.5436	1.05681E-08	3.01922E-08	5.13487E-04	-9.62E-09
NpO2OH (aq)	NpO2OH (aq)	9.21672E-09	1.09360E-09	0.1187	2.88822E-09	8.25141E-09	2.36035E-03	2.28E-09
NpO2 (CO3) 2=-	NpO2 (CO3) 2=-	1.59816E-09	3.31486E-13	2.0742E-04	5.00812E-10	1.43078E-09	5.56666E-04	-1.19E-08
NpO2 (CO3) 3=-	NpO2 (CO3) 3=-	2.16779E-13	7.99417E-22	3.6877E-09	6.79315E-14	1.94075E-13	8.71540E-08	-2.38E-08
NpO2 (OH) 2-	NpO2 (OH) 2-	5.83724E-14	1.18111E-15	2.0234E-02	1.82920E-14	5.22587E-14	1.58376E-08	-7.33E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31855E-01	7.78043E-01	0.9353	1.73954E+01	4.96952E+01	8.95269E+05
Na+	Na+	5.61001E+00	5.29025E+00	0.9430	1.75808E+00	5.02247E+00	1.15465E+05
Cl-	Cl-	5.60914E+00	5.29031E+00	0.9432	1.75781E+00	5.02169E+00	1.78034E+05
2 [NaNpO2CO3.7/2H2O(s)]		4.99767E+00	1.00000E+00	1.0000	1.56618E+00	4.47426E+00	3.71452E+06
HCO3-	HCO3-	8.83349E-04	3.27070E-04	0.3703	2.76826E-04	7.90835E-04	4.82545E+01
CO2 (aq)	CO2 (aq)	5.81133E-05	1.68731E-04	2.903	1.82117E-05	5.20270E-05	2.28970E+00
NpO2+	NpO2+	2.38788E-05	4.55721E-05	1.908	7.48319E-05	2.13779E-05	5.75167E+00
NpO2CO3-	NpO2CO3-	3.29745E-06	3.96256E-07	0.1202	1.03336E-06	2.95211E-06	9.71409E-01
CO3=	CO3=	3.12440E-06	8.11440E-08	2.5972E-02	9.79132E-07	2.79718E-06	1.67857E-01
OH-	OH-	7.81476E-08	4.24844E-08	0.5436	2.44900E-08	6.99631E-08	1.19888E-03
H+	H+	4.70737E-08	1.84550E-07	3.920	1.47520E-08	4.21436E-08	4.24765E-05
NpO2OH (aq)	NpO2OH (aq)	7.99163E-09	9.48305E-10	0.1187	2.50444E-09	7.15466E-09	2.04662E-03
NpO2 (CO3) 2=-	NpO2 (CO3) 2=-	4.27028E-09	8.85878E-13	2.0745E-04	1.33823E-09	3.82305E-09	1.48742E-03
NpO2 (CO3) 3=-	NpO2 (CO3) 3=-	1.54754E-12	5.70931E-21	3.6893E-09	4.84973E-13	1.38547E-12	6.22178E-07
NpO2 (OH) 2-	NpO2 (OH) 2-	1.17284E-13	2.37335E-15	2.0236E-02	3.67548E-14	1.05001E-13	3.18218E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31857E-01	7.78049E-01	0.9353	1.73964E+01	4.96953E+01	8.95271E+05
Na+	Na+	5.61000E+00	5.29002E+00	0.9430	1.75817E+00	5.02247E+00	1.15465E+05
Cl-	Cl-	5.60893E+00	5.29003E+00	0.9431	1.75783E+00	5.02151E+00	1.78028E+05
2 [NaNpO2CO3.7/2H2O(s)]		4.99741E+00	1.00000E+00	1.0000	1.56618E+00	4.47403E+00	3.71433E+06
HCO3-	HCO3-	9.89678E-04	3.66440E-04	0.3703	3.10165E-04	8.86030E-04	5.40630E+01
CO3=	CO3=	4.23895E-05	1.10096E-06	2.5972E-02	1.32848E-05	3.79501E-05	2.27735E+00
CO2 (aq)	CO2 (aq)	5.37651E-06	1.56106E-05	2.903	1.68500E-06	4.81344E-06	2.11838E-01
NpO2CO3-	NpO2CO3-	3.29722E-06	3.96261E-07	0.1202	1.03335E-06	2.95190E-06	9.71342E-01
NpO2+	NpO2+	1.76018E-06	3.35920E-06	1.908	5.51638E-07	1.57583E-06	4.23973E-01
OH-	OH-	9.46323E-07	5.14475E-07	0.5437	2.96577E-07	8.47215E-07	1.44088E-02
NpO2 (CO3) 2=-	NpO2 (CO3) 2=-	5.79268E-08	1.20191E-11	2.0749E-04	1.81542E-08	5.18601E-08	2.01770E-02
NpO2OH (aq)	NpO2OH (aq)	7.13261E-09	8.46441E-10	0.1187	2.23535E-09	6.38561E-09	1.82663E-03
H+	H+	3.88761E-09	1.52399E-08	3.920	1.21837E-09	3.48046E-09	3.50796E-06
NpO2 (CO3) 3=-	NpO2 (CO3) 3=-	2.84791E-10	1.05093E-18	3.6902E-09	8.92533E-11	2.54965E-10	1.14498E-04
NpO2 (OH) 2-	NpO2 (OH) 2-	1.26759E-12	2.56534E-14	2.0238E-02	3.97263E-13	1.13484E-12	3.43927E-07

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31858E-01	7.78055E-01	0.9353	1.73975E+01	4.96953E+01	8.95271E+05
Na+	Na+	5.61000E+00	5.28992E+00	0.9429	1.75829E+00	5.02247E+00	1.15466E+05
Cl-	Cl-	5.60866E+00	5.28964E+00	0.9431	1.75787E+00	5.02127E+00	1.78019E+05
2 [NaNpO2CO3.7/2H2O(s)]		4.99708E+00	1.00000E+00	1.0000	1.56618E+00	4.47374E+00	3.71409E+06
HCO3-	HCO3-	1.00032E-03	3.70372E-04	0.3703	3.13521E-04	8.95560E-04	5.46445E+01
CO3=	CO3=	1.67020E-04	4.33786E-06	2.5972E-02	5.23475E-05	1.49528E-04	8.97308E+00
OH-	OH-	3.68894E-06	2.00557E-06	0.5437	1.15619E-06	3.30261E-06	5.61684E-02
NpO2CO3-	NpO2CO3-	3.29692E-06	3.96259E-07	0.1202	1.03332E-06	2.95164E-06	9.71255E-01
CO2 (aq)	CO2 (aq)	1.39400E-06	4.04747E-06	2.903	4.36908E-07	1.24801E-06	5.49246E-02
NpO2+	NpO2+	4.46777E-07	8.52520E-07	1.908	1.40029E-07	3.99987E-07	1.07615E-01
NpO2 (CO3) 2=-	NpO2 (CO3) 2=-	2.28192E-07	4.73560E-11	2.0753E-04	7.15199E-08	2.04294E-07	7.94836E-02
NpO2OH (aq)	NpO2OH (aq)	7.05617E-09	8.37454E-10	0.1187	2.21155E-09	6.31719E-09	1.80706E-03
NpO2 (CO3) 3=-	NpO2 (CO3) 3=-	4.42139E-09	1.63148E-17	3.6900E-09	1.38575E-09	3.95834E-09	1.77759E-03
H+	H+	9.97385E-10	3.90943E-09	3.920	3.12600E-10	8.92930E-10	8.99984E-07
NpO2 (OH) 2-	NpO2 (OH) 2-	4.88845E-12	9.89424E-14	2.0240E-02	1.53214E-12	4.37649E-12	1.32635E-06

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31860E-01	7.78058E-01	0.9353	1.73984E+01	4.96953E+01	8.95272E+05
Na+	Na+	5.61000E+00	5.28986E+00	0.9429	1.75837E+00	5.02248E+00	1.15466E+05
Cl-	Cl-	5.60847E+00	5.28935E+00	0.9431	1.75789E+00	5.02110E+00	1.78013E+05
2 [NaNpO2CO3.7/2H2O(s)]		4.99683E+00	1.00000E+00	1.0000	1.56618E+00	4.47352E+00	3.71391E+06
HCO3-	HCO3-	1.00334E-03	3.71482E-04	0.3702	3.14482E-04	8.98260E-04	5.48092E+01
CO3=	CO3=	2.61433E-04	6.78989E-06	2.5972E-02	8.19423E-05	2.34053E-04	1.40454E+01
OH-	OH-	5.75685E-06	3.12987E-06	0.5437	1.80440E-06	5.15394E-06	8.76546E-02
NpO2CO3-	NpO2CO3-	3.29670E-06	3.96256E-07	0.1202	1.03330E-06	2.95144E-06	9.71191E-01
CO2 (aq)	CO2 (aq)	8.95926E-07	2.60132E-06	2.903	2.80815E-07	8.02097E-07	3.53001E-02
NpO2 (CO3) 2=-	NpO2 (CO3) 2=-	3.57129E-07	7.41241E-11	2.0756E-04	1.11937E-07	3.19728E-07	1.24395E-01
NpO2+	NpO2+	2.85452E-07	5.44647E-07	1.908	8.94709E-08	2.55557E-07	6.87569E-02
NpO2 (CO3) 3=-	NpO2 (CO3) 3=-	1.08331E-08	3.99718E-17	3.6898E-09	3.39549E-09	9.69860E-09	4.35539E-03
NpO2OH (aq)	NpO2OH (aq)	7.03457E-09	8.34952E-10	0.1187	2.20488E-09	6.29785E-09	1.80153E-03
H+	H+	6.39163E-10	2.50511E-09	3.919	2.00336E-10	5.72224E-10	5.76745E-07
NpO2 (OH) 2-	NpO2 (OH) 2-	7.60550E-12	1.53947E-13	2.0242E-02	2.36383E-12	6.80899E-12	2.06354E-06

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
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Figure 6.2.3 Edited Listing of the Output File FMT_NP_NACL_BM_QB0204.OUT
 (Page 4 of 4)

NpO2(OH)2- NpO2(OH)2- 6.20621E-11 1.25834E-12 2.0275E-02 1.94730E-11 5.55628E-11 1.68390E-05 -9.42E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.31928E-01	7.78275E-01	0.9355	1.74471E+01	4.96962E+01	8.95287E+05
Na+	Na+	5.61002E+00	5.28658E+00	0.9423	1.76330E+00	5.02258E+00	1.15468E+05
Cl-	Cl-	5.59730E+00	5.27271E+00	0.9420	1.75931E+00	5.01119E+00	1.77662E+05
2[NaNpO2CO3.7/2H2O(s)]		4.98287E+00	1.00000E+00	1.000	1.56618E+00	4.46110E+00	3.70360E+06
CO3=	CO3=	5.72079E-03	1.48479E-04	2.5954E-02	1.79812E-03	5.12175E-03	3.07352E+02
HCO3-	HCO3-	1.11030E-03	4.10631E-04	0.3698	3.48981E-04	9.94036E-04	6.06532E+01
OH-	OH-	1.13816E-04	6.19347E-05	0.5442	3.57739E-05	1.01898E-04	1.73301E+00
NpO2(CO3)2==	NpO2(CO3)2==	7.74613E-06	1.62034E-09	2.0918E-04	2.43471E-06	6.93501E-06	2.69817E+00
NpO2(CO3)3==	NpO2(CO3)3==	5.19587E-06	1.91075E-14	3.6774E-09	1.63313E-06	4.65180E-06	2.08900E+00
NpO2CO3-	NpO2CO3-	3.28419E-06	3.96116E-07	0.1206	1.03227E-06	2.94030E-06	9.67523E-01
CO2(aq)	CO2(aq)	5.00413E-08	1.45312E-07	2.904	1.57286E-08	4.48014E-08	1.97170E-03
NpO2+	NpO2+	1.31038E-08	4.48977E-08	1.900	4.11869E-09	1.17316E-08	3.15636E-03
NpO2OH(aq)	NpO2OH(aq)	6.33648E-09	7.55291E-10	0.1192	1.99164E-09	5.67297E-09	1.62278E-03
NpO2(OH)2-	NpO2(OH)2-	1.35543E-10	2.75570E-12	2.0331E-02	4.26030E-11	1.21350E-10	3.67766E-05
H+	H+	3.24654E-11	1.26631E-10	3.900	1.02043E-11	2.90658E-11	2.92955E-08
							3.20E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.32085E-01	7.78776E-01	0.9359	1.75603E+01	4.96980E+01	8.95320E+05
Na+	Na+	5.61008E+00	5.28011E+00	0.9412	1.77476E+00	5.02282E+00	1.15473E+05
Cl-	Cl-	5.57160E+00	5.23340E+00	0.9393	1.76259E+00	4.98837E+00	1.76853E+05
2[NaNpO2CO3.7/2H2O(s)]		4.95072E+00	1.00000E+00	1.000	1.56617E+00	4.43248E+00	3.67984E+06
CO3=	CO3=	1.82647E-02	4.73092E-04	2.5902E-02	5.77807E-03	1.63527E-02	9.81315E+02
HCO3-	HCO3-	1.30025E-03	4.79575E-04	0.3688	4.11338E-04	1.16414E-03	7.10326E+01
OH-	OH-	3.10136E-04	1.69080E-04	0.5452	9.81123E-05	2.77671E-04	4.72244E+00
NpO2(CO3)3==	NpO2(CO3)3==	5.31035E-05	1.93785E-13	3.6492E-09	1.67994E-05	4.75446E-05	2.13511E+01
NpO2(CO3)2==	NpO2(CO3)2==	2.42246E-05	5.15755E-09	2.1291E-04	7.66349E-06	2.16887E-05	8.43833E+00
NpO2CO3-	NpO2CO3-	3.25554E-06	3.95710E-07	0.1215	1.02990E-06	2.91475E-06	9.59118E-01
CO2(aq)	CO2(aq)	2.14022E-08	6.21653E-08	2.905	6.77064E-09	1.91619E-08	8.43309E-04
NpO2OH(aq)	NpO2OH(aq)	5.37076E-09	6.46462E-10	0.1204	1.69905E-09	4.80855E-09	1.37551E-03
NpO2+	NpO2+	4.14828E-09	7.80607E-09	1.882	1.31232E-09	3.71404E-09	9.99251E-04
NpO2(OH)2-	NpO2(OH)2-	3.13580E-10	6.43900E-12	2.0534E-02	9.92017E-11	2.80755E-10	8.50895E-05
H+	H+	1.20332E-11	4.64153E-11	3.857	3.80673E-12	1.07736E-11	1.08587E-08
							3.25E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.32536E-01	7.80198E-01	0.9371	1.78882E+01	4.97019E+01	8.95389E+05
Na+	Na+	5.61041E+00	5.26972E+00	0.9393	1.80801E+00	5.02350E+00	1.15489E+05
Cl-	Cl-	5.49894E+00	5.11550E+00	0.9303	1.77209E+00	4.92369E+00	1.74560E+05
2[NaNpO2CO3.7/2H2O(s)]		4.85974E+00	1.00000E+00	1.000	1.56610E+00	4.35136E+00	3.61249E+06
CO3=	CO3=	5.33144E-02	1.36866E-03	2.5671E-02	1.71811E-02	4.77371E-02	2.86467E+03
HCO3-	HCO3-	1.67388E-03	6.11619E-04	0.3655	5.39423E-04	1.49877E-03	9.14506E+01
OH-	OH-	7.01893E-04	3.84119E-04	0.5473	2.26192E-04	6.28468E-04	1.06885E+01
NpO2(CO3)3==	NpO2(CO3)3==	4.51984E-04	1.61474E-12	3.5726E-09	1.45656E-04	4.04702E-04	1.81741E+02
NpO2(CO3)2==	NpO2(CO3)2==	6.65320E-05	1.48551E-08	2.2328E-04	2.14406E-05	5.95721E-05	2.31774E+01
NpO2CO3-	NpO2CO3-	3.17561E-06	3.93967E-07	0.1241	1.02337E-06	2.84340E-06	9.35639E-01
CO2(aq)	CO2(aq)	1.20090E-08	3.49091E-08	2.907	3.87002E-09	1.07527E-08	4.73226E-04
NpO2OH(aq)	NpO2OH(aq)	4.08463E-09	5.05419E-10	0.1237	1.31631E-09	3.65733E-09	1.04620E-03
NpO2+	NpO2+	1.46743E-09	2.68637E-09	1.831	4.72896E-10	1.31393E-09	3.53508E-04
NpO2(OH)2-	NpO2(OH)2-	5.42276E-10	1.14367E-11	2.1090E-02	1.74754E-10	4.85548E-10	1.47151E-04
H+	H+	5.47721E-12	2.04682E-11	3.737	1.76509E-12	4.90423E-12	4.94298E-09
							5.43E-10

Total G/RT= -5.28148539E+03
 TITRATE file name is WFSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_NP_NACL_BM_QB0204.TITRATE;1

Figure 6.2.4 Edited Listing of the Output File FMT_NP_NACL_BM_QB0204.TITRATE
 (Page 1 of 2)

Benchmark TITRATE Problem; Np(V)O2 with CO3 in 5.61molal NaCl FMT V2.4
 FMT_ph_970407.chemdat
 Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5=== by analogy

Titration Results, molal

CO3=

- 1.08181E-07
- 3.54871E-07
- 1.16916E-06
- 3.12440E-06
- 4.23895E-05
- 1.67020E-04
- 2.61433E-04
- 3.73509E-04
- 4.85733E-04
- 6.50970E-04
- 1.34191E-03
- 2.32616E-03
- 5.72079E-03
- 1.82647E-02
- 5.33144E-02

	NpO2+	NpO2CO3-	NpO2 (CO3) 2=-	NpO2 (CO3) 3=-	NpO2OH(aq)	NpO2 (OH) 2-
0)	6.89566E-04	3.29958E-06	1.48074E-10	1.86478E-15	1.86099E-08	2.20062E-14
1)	2.10212E-04	3.29820E-06	4.85263E-10	1.99953E-14	1.23582E-08	3.18488E-14
2)	6.38093E-05	3.29766E-06	1.59816E-09	2.16779E-13	9.21672E-09	5.83724E-14
3)	2.38788E-05	3.29745E-06	4.27028E-09	1.54754E-12	7.99163E-09	1.17284E-13
4)	1.76018E-06	3.29722E-06	5.79268E-08	2.84791E-10	7.13261E-09	1.26759E-12
5)	4.46777E-07	3.29692E-06	2.28192E-07	4.42139E-09	7.05617E-09	4.88845E-12
6)	2.85452E-07	3.29670E-06	3.57129E-07	1.08331E-08	7.03457E-09	7.60550E-12
7)	1.99817E-07	3.29645E-06	5.10138E-07	2.21132E-08	7.01371E-09	1.08025E-11
8)	1.53665E-07	3.29619E-06	6.63293E-07	3.73990E-08	6.99472E-09	1.39733E-11
9)	1.14676E-07	3.29581E-06	8.88696E-07	6.71753E-08	6.96833E-09	1.85878E-11
10)	5.56616E-08	3.29422E-06	1.82992E-06	2.85516E-07	6.86602E-09	3.72177E-11
11)	3.21359E-08	3.29197E-06	3.16708E-06	8.58217E-07	6.73190E-09	6.20621E-11
12)	1.31038E-08	3.28419E-06	7.74613E-06	5.19587E-06	6.33648E-09	1.35543E-10
13)	4.14828E-09	3.25554E-06	2.42246E-05	5.31035E-05	5.37076E-09	3.13580E-10
14)	1.46743E-09	3.17561E-06	6.65320E-05	4.51984E-04	4.08463E-09	5.42276E-10
15)						

- 0) 2[NaNpO2CO3.7
- 1) 4.99941E+00
- 2) 4.99837E+00
- 3) 4.99788E+00
- 4) 4.99767E+00
- 5) 4.99741E+00
- 6) 4.99708E+00
- 7) 4.99683E+00
- 8) 4.99655E+00
- 9) 4.99626E+00
- 10) 4.99584E+00
- 11) 4.99407E+00
- 12) 4.99155E+00
- 13) 4.98287E+00
- 14) 4.95072E+00
- 15) 4.85974E+00

	IonicStrength	Titrvol,ml	pH	pmH
0)	5.61111E+00	0.000000000E+00	5.640	6.234
1)	5.61033E+00	0.100000000	5.978	6.572
2)	5.61010E+00	0.142510000	6.369	6.962
3)	5.61004E+00	0.160000000	6.734	7.327
4)	5.61005E+00	0.180000000	7.817	8.410
5)	5.61017E+00	0.203090000	8.408	9.001
6)	5.61027E+00	0.220000000	8.601	9.194
7)	5.61038E+00	0.240000000	8.755	9.348
8)	5.61049E+00	0.260000000	8.868	9.461
9)	5.61066E+00	0.289430000	8.993	9.586
10)	5.61136E+00	0.412460000	9.301	9.894
11)	5.61235E+00	0.587800000	9.532	10.12
12)	5.61582E+00	1.19380000	9.897	10.49
13)	5.62895E+00	3.45510000	10.33	10.92
14)	5.66844E+00	10.000000	10.69	11.26
15)				

6.2.4 Evaluation

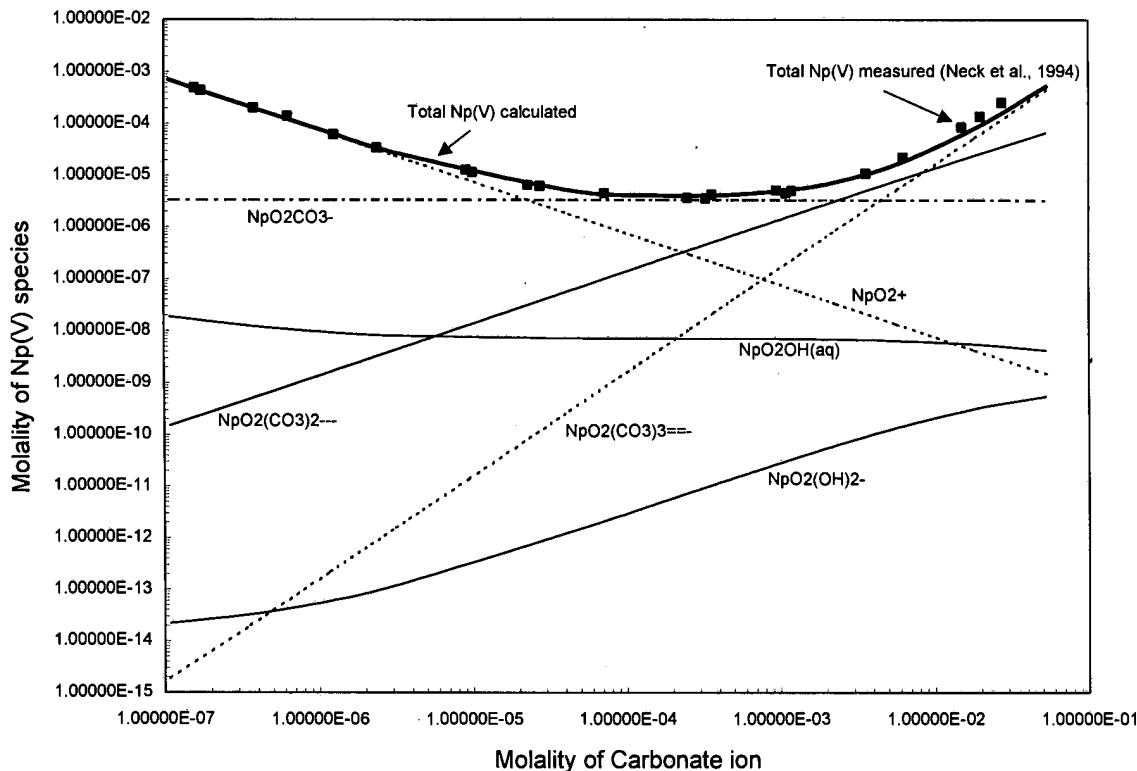
The calculated Np solubility was to be compared with the experimental data from Neck et al. (1994) (Table 6.2.1). The model prediction was expected to follow the general trend of the experimental data and the deviation of the model prediction from the experimental data was to be less than half a logarithmic unit to be acceptable.

Table 6.2.1
Experimental Measurements from Neck et al. (1994)

m CO ₃ ²⁻	mNp(V) total		m CO ₃ ²⁻	mNp(V) total
9.49E-4	5.13E-6		3.61E-3	1.07E-5
3.61E-4	4.17E-6		6.27E-3	2.24E-5
7.20E-5	4.47E-6		1.50E-2	8.51E-5
9.93E-6	1.15E-5		1.98E-2	1.38E-4
2.38E-6	3.39E-5		2.74E-2	2.57E-4
1.25E-6	6.17E-5		1.09E-3	4.47E-6
3.78E-7	2.04E-4		3.29E-4	3.55E-6
1.73E-7	4.37E-4		2.50E-4	3.63E-6
1.57E-7	4.90E-4		2.28E-5	6.46E-6
9.06E-6	1.29E-5		6.27E-7	1.41E-4
2.74E-5	6.17E-6		5.72E-8	1.10E-3
1.19E-3	4.90E-6			

Since the m CO₃²⁻ values for the Neck data and the calculated results from FMT were not identical, comparison was made graphically. Figure 6.2.3 shows the output file FMT_NP_NACL_BM_QB0204.OUT edited to show the nonzero concentrations calculated by FMT. Figure 6.2.4 shows the nonzero titration results calculated by FMT. Both output files have been retained unedited in CMS.

Figure 6.2.5 Graphical Comparison of Total Np(V) Species Concentrations as a Function of CO_2^{3-} in 5.61 Molal NaCl with Experimental Measurements from Neck et al. (1994)



The graphical comparison in **Figure 6.2.5** shows that the calculated values follow the general trend of the experimental data (Neck, 1994). The deviation of the model prediction from the experimental data was shown to be less than half a logarithmic. The acceptance criteria is considered to have been met.

6.3 Test Case #3: ThO₂ (am) Solubility in 6 m NaCl Solution

6.3.1 Test Objectives

This test case used the "titration" mode of logarithmic increments to calculate the solubility of ThO₂ (am) in a 6 m NaCl solution as a function of pcH (= log[molarity of H⁺]). This test case was intended to ascertain if FMT correctly predicts the chemical behavior of Th(IV) in NaCl solutions. It tests functional requirements R.2, R.4, and R.7.

6.3.2 Test Procedures

This test case was run using the script FMT_TEST_QB0204.COM. This command file is shown in **Figure 6.0.2**.

6.3.3 Input/Output Files

The following is a list of all files associated with Test Case #1:

Command file:

FMT_TEST_QB0204.COM

Input files:

FMT_THO2_6MNACL.IN

(See **Figure 6.3.1**)

FMT_THO2_6MNACL.INGUESS

(See **Figure 6.3.2**)

Output files:

FMT_THO2_6MNACL_QB0204.OUT

(See **Figure 6.3.3**)

FMT_THO2_6MNACL_QB0204.TITRATE

(See **Figure 6.3.4**)

Figure 6.3.1 Listing of the Input File FMT_THO2_6MNAACL.IN
(Page 1 of 2)

```
'FMT Test Case: Solubility of ThO2(am) in 6m NaCl'  
'CHEMFILE'  
'TITRATE' 'EXPLICIT'  
'DISABLE SPECIES' 0  
'nSET_FC02' 0.0  
'nSET_PH' 0.0
```

```
'nMOLES' 'nEXACT'  pmH=3.8  
1.11117763E+02  Hydrogen  
5.57090817E+01  Oxygen  
5.90000000E+00  Sodium  
0.00000000E+00  Potassium  
0.00000000E+00  Magnesium  
0.00000000E+00  Calcium  
6.00000000E+00  Chlorine  
0.00000000E+00  Sulfur  
0.00000000E+00  Carbon  
0.00000000E+00  PosIon:EL  
0.00000000E+00  NegIon:EL  
0.00000000E+00  Oxalate:EL  
0.00000000E+00  Boron  
0.00000000E+00  Bromine  
0.00000000E+00  Acetate:EL  
1.00100000E-01  Th(IV)  
0.00000000E+00  Am(III)  
0.00000000E+00  U(VI)  
0.00000000E+00  Np(V)  
0.00000000E+00  ClO4:EL  
0.00000000E+00  Phosphorus  
0.00000000E+00  U(IV)  
0.00000000E+00  Lactate:EL  
0.00000000E+00  EDTA:EL  
0.00000000E+00  Citrate:EL  
0.00000000E+00  Electron:E  
0.00000000E+00  Charge:EL
```

```
'nMOLES' 'nEXACT'  pmH=5.5  
9.75240060E+01  Hydrogen  
4.89378653E+01  Oxygen  
5.27072240E+00  Sodium  
0.00000000E+00  Potassium  
0.00000000E+00  Magnesium  
0.00000000E+00  Calcium  
5.27072516E+00  Chlorine  
0.00000000E+00  Sulfur  
0.00000000E+00  Carbon  
0.00000000E+00  PosIon:EL  
0.00000000E+00  NegIon:EL  
0.00000000E+00  Oxalate:EL  
0.00000000E+00  Boron  
0.00000000E+00  Bromine  
0.00000000E+00  Acetate:EL  
8.79318365E-02  Th(IV)  
0.00000000E+00  Am(III)  
0.00000000E+00  U(VI)  
0.00000000E+00  Np(V)  
0.00000000E+00  ClO4:EL  
0.00000000E+00  Phosphorus  
0.00000000E+00  U(IV)  
0.00000000E+00  Lactate:EL  
0.00000000E+00  EDTA:EL  
0.00000000E+00  Citrate:EL  
0.00000000E+00  Electron:E  
0.00000000E+00  Charge:EL
```

```
16 2.25d3 0.0025d0 1.800001d5 'ndxVARIABLE'  
'nDIFFUS'  
'CONVEC'
```

Figure 6.3.1 Listing of the Input File FMT_THO2_6MNACL.IN
(Page 2 of 2)

```
'nSSDIFF'  
'nRESTART'  
'nPUSHPULL' 'nMULTINJ'  
  
20 1 20 'nLOTS' 10  
'nTGRAD' 'LINEAR'  
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'  
3  
0.1d0 0.2d0 0.3d0  
1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF' vfrc dfrc FPOR mpor dmxt  
'nMOLES' 'nEXACT' Plain old pure H2O  
1.11017360E+02 Hydrogen  
5.55086800E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL  
  
1.d-12 1.d-20 (fracture matrix permeabilities)  
'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH default is all flash)  
'VAR_AQ_RHO' 1074.9d0  
'nNO X DIFF'  
'UNIFORM' 0  
  
'TITRATE' 'LOG10' 0.01 2000.0 'nINJSOLIDS'
```

Figure 6.3.2 Listing of the Input File FMT_THO2_6MNACL.INGUESS

(This file is necessary but is intentionally blank for this test case.)

Figure 6.3.3 Edited Listing of the Output File FMT_THO2_6MNAACL_QB0204.OUT
 (Page 1 of 3)

NPWT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_THO2_6MNAACL.IN:1
 INGUSS file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_THO2_6MNAACL.INGUSS:1
 OUTPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_THO2_6MNAACL_QB0204.OUT:1
 CHEMDAT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT:1
 Temperature is Hard Coded as 298.15K
 FMT Test Case: Solubility of ThO2(am) in 6m NaCl FMT V2.4
 FMT_ph 970407.chemdat
 Added Th(CO3)5-Cl(-Na) Parmas, assigned K+-Th(CO3)5=== by analogy

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.23289E-01	7.55084E-01	0.9172	5.55588E+01	4.92836E+01	8.87855E+05
Cl-	Cl-	5.99459E+00	6.42956E+00	1.073	6.00000E+00	5.32232E+00	1.88692E+05
Na+	Na+	5.89468E+00	5.76342E+00	0.9777	5.90000E+00	5.23362E+00	1.20320E+05
ThO2(am) _____Hydrous_Thorium_Oxide		7.50723E-02	1.00000E+00	1.000	7.51401E-02	6.66533E-02	1.75989E+04
Th++++	Th++++	2.49374E-02	1.52060E-02	0.6098	2.49599E-02	2.21408E-02	5.13750E+03
H+	H+	1.60202E-04	7.29260E-04	4.552	1.60347E-04	1.42236E-04	1.43360E-01
Th(OH)4(aq)	Th(OH)4(aq)	1.30527E-09	1.30527E-09	1.000	1.30645E-09	1.15889E-09	3.47746E-04
OH-	OH-	1.97257E-11	1.04341E-11	0.5290	1.97435E-11	1.75136E-11	2.97859E-07

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22246E-01	7.59249E-01	0.9234	4.87620E+01	4.93337E+01	8.88756E+05
Cl-	Cl-	5.99998E+00	5.94696E+00	0.9912	5.27073E+00	5.33252E+00	1.89054E+05
Na+	Na+	5.99998E+00	5.94695E+00	0.9912	5.27072E+00	5.33251E+00	1.22593E+05
ThO2(am) _____Hydrous_Thorium_Oxide		1.00098E-01	1.00000E+00	1.000	8.79318E-02	8.89627E-02	2.34894E+04
H+	H+	3.13043E-06	1.40714E-05	4.495	2.74995E-06	2.78219E-06	2.80417E-03
Th++++	Th++++	3.10808E-09	2.08477E-09	0.6708	2.73032E-09	2.76232E-09	6.40965E-04
OH-	OH-	9.95011E-10	5.43734E-10	0.5465	8.74074E-10	8.84321E-10	1.50399E-05
Th(OH)4(aq)	Th(OH)4(aq)	1.31972E-09	1.31972E-09	1.000	1.15931E-09	1.17290E-09	3.51950E-04

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22246E-01	7.59249E-01	0.9234	4.87610E+01	4.93337E+01	8.88756E+05
Cl-	Cl-	5.99998E+00	5.94696E+00	0.9912	5.27061E+00	5.33252E+00	1.89054E+05
Na+	Na+	5.99998E+00	5.94695E+00	0.9912	5.27061E+00	5.33251E+00	1.22593E+05
ThO2(am) _____Hydrous_Thorium_Oxide		1.00098E-01	1.00000E+00	1.000	8.79300E-02	8.89627E-02	2.34894E+04
H+	H+	3.13043E-06	1.40714E-05	4.495	2.74989E-06	2.78219E-06	2.80417E-03
Th++++	Th++++	3.10808E-09	2.08477E-09	0.6708	2.73026E-09	2.76232E-09	6.40965E-04
Th(OH)4(aq)	Th(OH)4(aq)	1.31972E-09	1.31972E-09	1.000	1.15929E-09	1.17290E-09	3.51950E-04
OH-	OH-	9.95011E-10	5.43734E-10	0.5465	8.74056E-10	8.84321E-10	1.50399E-05

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22246E-01	7.59249E-01	0.9234	4.87615E+01	4.93337E+01	8.88756E+05
Cl-	Cl-	5.99998E+00	5.94696E+00	0.9912	5.27067E+00	5.33252E+00	1.89054E+05
Na+	Na+	5.99998E+00	5.94695E+00	0.9912	5.27066E+00	5.33251E+00	1.22593E+05
ThO2(am) _____Hydrous_Thorium_Oxide		1.00097E-01	1.00000E+00	1.000	8.79302E-02	8.89620E-02	2.34893E+04
H+	H+	4.11526E-06	1.84983E-05	4.495	3.61504E-06	3.65746E-06	3.68636E-03
Th++++	Th++++	9.28248E-09	6.22632E-09	0.6708	8.15417E-09	8.24986E-09	1.91428E-03
Th(OH)4(aq)	Th(OH)4(aq)	1.31972E-09	1.31972E-09	1.000	1.15930E-09	1.17290E-09	3.51950E-04
OH-	OH-	7.56894E-10	4.13612E-10	0.5465	6.64891E-10	6.72693E-10	1.14407E-05

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22246E-01	7.59249E-01	0.9234	4.87621E+01	4.93337E+01	8.88756E+05
Cl-	Cl-	5.99998E+00	5.94696E+00	0.9912	5.27074E+00	5.33252E+00	1.89054E+05
Na+	Na+	5.99997E+00	5.94695E+00	0.9912	5.27074E+00	5.33251E+00	1.22593E+05
ThO2(am) _____Hydrous_Thorium_Oxide		1.00096E-01	1.00000E+00	1.000	8.79305E-02	8.89610E-02	2.34890E+04
H+	H+	5.44346E-06	2.44686E-05	4.495	4.78186E-06	4.83790E-06	4.87612E-03
Th++++	Th++++	2.84166E-08	1.90670E-08	0.6708	2.49628E-08	2.52554E-08	5.86021E-03
Th(OH)4(aq)	Th(OH)4(aq)	1.31971E-09	1.31971E-09	1.000	1.15932E-09	1.17290E-09	3.51950E-04
OH-	OH-	5.72213E-10	3.12692E-10	0.5465	5.02666E-10	5.08558E-10	8.64919E-06

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22246E-01	7.59249E-01	0.9234	4.87638E+01	4.93337E+01	8.88756E+05
Cl-	Cl-	5.99998E+00	5.94697E+00	0.9912	5.27092E+00	5.33252E+00	1.89054E+05
Na+	Na+	5.99997E+00	5.94695E+00	0.9912	5.27091E+00	5.33251E+00	1.22593E+05
ThO2(am) _____Hydrous_Thorium_Oxide		1.00094E-01	1.00000E+00	1.000	8.79311E-02	8.89587E-02	2.34884E+04
H+	H+	8.30157E-06	3.73159E-05	4.495	7.29284E-06	7.37806E-06	7.43635E-03
Th++++	Th++++	1.53713E-07	1.03105E-07	0.6708	1.35035E-07	1.36613E-07	3.16995E-02
Th(OH)4(aq)	Th(OH)4(aq)	1.31971E-09	1.31971E-09	1.000	1.15936E-09	1.17290E-09	3.51950E-04
OH-	OH-	3.75209E-10	2.05036E-10	0.5465	3.29617E-10	3.33469E-10	5.67140E-06

Figure 6.3.3 Edited Listing of the Output File FMT_THO2_6MNAACL_QB0204.OUT
 (Page 2of 3)

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22246E-01	7.59249E-01	0.9234	4.87677E+01	4.93337E+01	8.88756E+05	
Cl-	Cl-	5.99998E+00	5.94699E+00	0.9912	5.27134E+00	5.33252E+00	1.89054E+05	
Na+	Na+	5.99996E+00	5.94694E+00	0.9912	5.27133E+00	5.33250E+00	1.22593E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	1.00087E-01	1.00000E+00	1.0000	8.79322E-02	8.89526E-02	2.34868E+04	
H+	H+	1.31169E-05	5.89609E-05	4.495	1.15240E-05	1.16577E-05	1.17498E-02	
Th++++	Th++++	9.58060E-07	6.42634E-07	0.6708	8.41713E-07	8.51481E-07	1.97576E-01	1.73E-08
Th(OH) 4 (aq)	Th(OH) 4 (aq)	1.31971E-09	1.31971E-09	1.0000	1.15945E-09	1.17290E-09	3.51950E-04	-7.41E-14
OH-	OH-	2.37467E-10	1.29766E-10	0.5465	2.08629E-10	2.11050E-10	3.58939E-06	-2.41E-07

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22246E-01	7.59248E-01	0.9234	4.87771E+01	4.93336E+01	8.88756E+05	
Cl-	Cl-	5.99998E+00	5.94706E+00	0.9912	5.27235E+00	5.33251E+00	1.89054E+05	
Na+	Na+	5.99994E+00	5.94691E+00	0.9912	5.27232E+00	5.33248E+00	1.22593E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	1.00069E-01	1.00000E+00	1.0000	8.79335E-02	8.89368E-02	2.34827E+04	
H+	H+	1.90617E-05	8.56832E-05	4.495	1.67501E-05	1.69412E-05	1.70750E-02	
Th++++	Th++++	4.27289E-06	2.86609E-06	0.6708	3.75471E-06	3.79755E-06	8.81176E-01	-7.26E-10
Th(OH) 4 (aq)	Th(OH) 4 (aq)	1.31971E-09	1.31971E-09	1.0000	1.15967E-09	1.17290E-09	3.51949E-04	-2.47E-14
OH-	OH-	1.63408E-10	8.92952E-11	0.5465	1.43591E-10	1.45230E-10	2.46997E-06	-2.14E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22246E-01	7.59247E-01	0.9234	4.87995E+01	4.93336E+01	8.88755E+05	
Cl-	Cl-	5.99998E+00	5.94725E+00	0.9912	5.27478E+00	5.33251E+00	1.89053E+05	
Na+	Na+	5.99998E+00	5.94683E+00	0.9912	5.27470E+00	5.33244E+00	1.22592E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	1.00025E-01	1.00000E+00	1.0000	8.79349E-02	8.88974E-02	2.34722E+04	
H+	H+	2.56865E-05	1.15463E-04	4.495	2.25819E-05	2.28290E-05	2.30094E-02	
Th++++	Th++++	1.40902E-05	9.45094E-06	0.6707	1.23872E-05	1.25228E-05	2.90576E+00	-1.28E-09
Th(OH) 4 (aq)	Th(OH) 4 (aq)	1.31971E-09	1.31971E-09	1.0000	1.16020E-09	1.17290E-09	3.51947E-04	2.47E-14
OH-	OH-	1.21264E-10	6.62646E-11	0.5464	1.06607E-10	1.07774E-10	1.83295E-06	-3.16E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22247E-01	7.59242E-01	0.9234	4.88531E+01	4.93336E+01	8.88754E+05	
Cl-	Cl-	5.99997E+00	5.94774E+00	0.9913	5.28057E+00	5.33250E+00	1.89053E+05	
Na+	Na+	5.99978E+00	5.94663E+00	0.9911	5.28040E+00	5.33233E+00	1.22589E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	9.99167E-02	1.00000E+00	1.0000	8.79365E-02	8.88014E-02	2.34468E+04	
Th++++	Th++++	3.95926E-05	2.65544E-05	0.6707	3.48454E-05	3.51881E-05	8.16499E+00	
H+	H+	3.32555E-05	1.49488E-04	4.495	2.92682E-05	2.95560E-05	2.97895E-02	-1.80E-11
Th(OH) 4 (aq)	Th(OH) 4 (aq)	1.31969E-09	1.31969E-09	1.0000	1.16146E-09	1.17288E-09	3.51943E-04	2.47E-14
OH-	OH-	9.36659E-11	5.11817E-11	0.5464	8.24353E-11	8.32460E-11	1.15479E-06	-7.86E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22250E-01	7.59231E-01	0.9234	4.89814E+01	4.93335E+01	8.88752E+05	
Cl-	Cl-	5.99996E+00	5.94894E+00	0.9915	5.29442E+00	5.33247E+00	1.89052E+05	
Na+	Na+	5.99950E+00	5.94615E+00	0.9911	5.29402E+00	5.33207E+00	1.22583E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	9.96572E-02	1.00000E+00	1.0000	8.79384E-02	8.85706E-02	2.33859E+04	
Th++++	Th++++	1.02626E-04	6.88152E-05	0.6705	9.05579E-05	9.12088E-05	2.11639E+01	
H+	H+	4.21925E-05	1.89666E-04	4.495	3.72310E-05	3.74986E-05	3.77949E-02	-6.05E-12
Th(OH) 4 (aq)	Th(OH) 4 (aq)	1.31965E-09	1.31965E-09	1.0000	1.16447E-09	1.17284E-09	3.51932E-04	0.00E+00
OH-	OH-	7.38291E-11	4.03390E-11	0.5464	6.51475E-11	6.56158E-11	1.11595E-06	-1.73E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22256E-01	7.59205E-01	0.9233	4.92880E+01	4.93332E+01	8.88747E+05	
Cl-	Cl-	5.99992E+00	5.95183E+00	0.9920	5.32753E+00	5.33241E+00	1.89050E+05	
Na+	Na+	5.99885E+00	5.94500E+00	0.9910	5.32658E+00	5.33146E+00	1.22569E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	9.90397E-02	1.00000E+00	1.0000	8.79407E-02	8.80212E-02	2.32408E+04	
Th++++	Th++++	2.54639E-04	1.70656E-04	0.6702	2.26102E-04	2.26309E-04	5.25124E+01	
H+	H+	5.29425E-05	2.38008E-04	4.496	4.70094E-05	4.70525E-05	4.74242E-02	-2.30E-12
Th(OH) 4 (aq)	Th(OH) 4 (aq)	1.31956E-09	1.31956E-09	1.0000	1.17168E-09	1.17276E-09	3.51906E-04	0.00E+00
OH-	OH-	5.88434E-11	3.21446E-11	0.5463	5.22491E-11	5.22969E-11	8.89429E-07	-3.80E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22271E-01	7.59144E-01	0.9232	5.00213E+01	4.93324E+01	8.88734E+05	
Cl-	Cl-	5.99985E+00	5.95864E+00	0.9931	5.40673E+00	5.33227E+00	1.89045E+05	
Na+	Na+	5.99733E+00	5.94228E+00	0.9908	5.40446E+00	5.33003E+00	1.22536E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	9.75906E-02	1.00000E+00	1.0000	8.79432E-02	8.67321E-02	2.29005E+04	
Th++++	Th++++	6.13646E-04	4.10733E-04	0.6693	5.52983E-04	5.45368E-04	1.26546E+02	
H+	H+	6.59281E-05	2.96438E-04	4.496	5.94107E-05	5.89525E-05	5.90554E-02	-9.38E-13
Th(OH) 4 (aq)	Th(OH) 4 (aq)	1.31935E-09	1.31935E-09	1.0000	1.18892E-09	1.17255E-09	3.51844E-04	2.47E-14
OH-	OH-	4.72634E-11	2.58066E-11	0.5460	4.25912E-11	4.20046E-11	7.14385E-07	-8.26E-12

Figure 6.3.3 Edited Listing of the Output File FMT_THO2_6MNAQL_QB0204.OUT
 (Page 3of 3)

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22306E-01	7.59004E-01	0.9230	5.17750E+01	4.93308E+01	8.88704E+05	
Cl-	Cl-	5.99967E+00	5.97421E+00	0.9958	5.59611E+00	5.33193E+00	1.89033E+05	
Na+	Na+	5.99885E+00	5.93609E+00	0.9904	5.59069E+00	5.32676E+00	1.22461E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	9.42882E-02	1.00000E+00	1.000	8.79461E-02	8.37943E-02	2.21248E+04	
Th++++	Th++++	1.43444E-03	9.57291E-04	0.6674	1.33795E-03	1.27479E-03	2.95800E+02	
H+	H+	8.14193E-05	3.66239E-04	4.498	7.59428E-05	7.23577E-05	7.29293E-02	-3.95E-13
Th(OH)4 (aq)	Th(OH)4 (aq)	1.31886E-09	1.31886E-09	1.000	1.23015E-09	1.17208E-09	3.51702E-04	4.94E-14
OH-	OH-	3.82895E-11	2.08843E-11	0.5454	3.57140E-11	3.40280E-11	5.78725E-07	-1.97E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22379E-01	7.58705E-01	0.9226	5.59686E+01	4.93273E+01	8.88641E+05	
Cl-	Cl-	5.99929E+00	6.00762E+00	1.001	6.04900E+00	5.33121E+00	1.89007E+05	
Na+	Na+	5.98642E+00	5.92288E+00	0.9894	6.03603E+00	5.31978E+00	1.22300E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	8.72263E-02	1.00000E+00	1.000	8.79491E-02	7.75128E-02	2.04662E+04	
Th++++	Th++++	3.19252E-03	2.11702E-03	0.6631	3.21897E-03	2.83700E-03	6.58292E+02	
H+	H+	9.91830E-05	4.46528E-04	4.502	1.00005E-04	8.81380E-05	8.88343E-02	-1.67E-13
Th(OH)4 (aq)	Th(OH)4 (aq)	1.31782E-09	1.31782E-09	1.000	1.32874E-09	1.17107E-09	3.51400E-04	-2.47E-14
OH-	OH-	3.14644E-11	1.71224E-11	0.5442	3.17251E-11	2.79605E-11	4.75533E-07	-7.22E-13

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22517E-01	7.58146E-01	0.9217	6.59972E+01	4.93206E+01	8.88521E+05	
Cl-	Cl-	5.99858E+00	6.07065E+00	1.012	7.13202E+00	5.32986E+00	1.88960E+05	
Na+	Na+	5.97248E+00	5.89820E+00	0.9876	7.10099E+00	5.30667E+00	1.21999E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	7.39743E-02	1.00000E+00	1.000	8.79519E-02	6.57277E-02	1.73545E+04	
Th++++	Th++++	6.49439E-03	4.25452E-03	0.6551	7.72152E-03	5.77040E-03	1.33895E+03	
H+	H+	1.17855E-04	5.31460E-04	4.509	1.40124E-04	1.04717E-04	1.05544E-01	-7.41E-14
Th(OH)4 (aq)	Th(OH)4 (aq)	1.31588E-09	1.31588E-09	1.000	1.56452E-09	1.16919E-09	3.50835E-04	0.00E+00
OH-	OH-	2.65307E-11	1.43755E-11	0.5418	3.15437E-11	2.35731E-11	4.00914E-07	-7.47E-13

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22723E-01	7.57320E-01	0.9205	8.99790E+01	4.93108E+01	8.88344E+05	
Cl-	Cl-	5.99751E+00	6.16515E+00	1.028	9.72191E+00	5.32785E+00	1.88888E+05	
Na+	Na+	5.95174E+00	5.86179E+00	0.9849	9.64771E+00	5.28719E+00	1.21551E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	5.42595E-02	1.00000E+00	1.000	8.79541E-02	4.82011E-02	1.27269E+04	
Th++++	Th++++	1.14086E-02	7.33690E-03	0.6431	1.84932E-02	1.01347E-02	2.35164E+03	
H+	H+	1.34650E-04	6.08694E-04	4.521	2.18267E-04	1.19616E-04	1.20561E-01	-3.70E-14
Th(OH)4 (aq)	Th(OH)4 (aq)	1.31302E-09	1.31302E-09	1.000	2.12839E-09	1.16641E-09	3.50001E-04	-4.94E-14
OH-	OH-	2.32879E-11	1.25378E-11	0.5384	3.77494E-11	2.06876E-11	3.51840E-07	-3.18E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.22943E-01	7.56443E-01	0.9192	1.47328E+02	4.93002E+01	8.88153E+05	
Cl-	Cl-	5.99637E+00	6.26731E+00	1.045	1.59153E+01	5.32570E+00	1.88812E+05	
Na+	Na+	5.92953E+00	5.82318E+00	0.9821	1.57378E+01	5.26633E+00	1.21072E+05	
ThO2 (am)	Hydrous_Thorium_Oxide	3.31389E-02	1.00000E+00	1.000	8.79556E-02	2.94324E-02	7.77125E+03	
Th++++	Th++++	1.66743E-02	1.05076E-02	0.6302	4.42559E-02	1.48093E-02	3.46332E+03	
H+	H+	1.46822E-04	6.65495E-04	4.533	3.89687E-04	1.30400E-04	1.31430E-01	-1.85E-14
Th(OH)4 (aq)	Th(OH)4 (aq)	1.30998E-09	1.30998E-09	1.000	3.47687E-09	1.16346E-09	3.49116E-04	2.47E-14
OH-	OH-	2.14222E-11	1.14544E-11	0.5347	5.68578E-11	1.90262E-11	3.23585E-07	-8.65E-11

Total G/RT= -1.66361139E+04
 TITRATE file name is WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_THO2_6MNAQL_QB0204.TITRATE;1

Figure 6.3.4 Edited Listing of the Output File FMT_THO2_6MNAACL_QB0204.TITRATE
(Page 1 of 2)

FMT Test Case: Solubility of ThO₂(am) in 6m NaCl
FMT pH_970407.chemdat
Added Th(CO₃)₅-Cl(-Na) Parm, assigned K+-Th(CO₃)₅=== by analogy

FMT V2.4

Titrant Volumes per Grid Block, in milliliters

1	0.000000 mL
2	0.010000 mL
3	0.023914 mL
4	0.057186 mL
5	0.136752 mL
6	0.327024 mL
7	0.782033 mL
8	1.870122 mL
9	4.472136 mL
10	10.694488 mL
11	25.574373 mL
12	61.157538 mL
13	146.249704 mL
14	349.735724 mL
15	836.344097 mL
16	2000.000000 mL

Titration Results, molal

0)	H2O	Na+	H+	Cl-
1)	4.87610E+01	5.99998E+00	3.13043E-06	5.99998E+00
2)	4.87615E+01	5.99998E+00	4.11526E-06	5.99998E+00
3)	4.87621E+01	5.99997E+00	5.44346E-06	5.99998E+00
4)	4.87638E+01	5.99997E+00	8.30157E-06	5.99998E+00
5)	4.87677E+01	5.99996E+00	1.31169E-05	5.99998E+00
6)	4.87771E+01	5.99994E+00	1.90617E-05	5.99998E+00
7)	4.87995E+01	5.99989E+00	2.56865E-05	5.99998E+00
8)	4.88531E+01	5.99978E+00	3.32555E-05	5.99997E+00
9)	4.89814E+01	5.99950E+00	4.21925E-05	5.99996E+00
10)	4.92880E+01	5.99885E+00	5.29425E-05	5.99992E+00
11)	5.00213E+01	5.99733E+00	6.59281E-05	5.99985E+00
12)	5.17750E+01	5.99385E+00	8.14193E-05	5.99967E+00
13)	5.59686E+01	5.98642E+00	9.91830E-05	5.99929E+00
14)	6.59972E+01	5.97248E+00	1.17855E-04	5.99858E+00
15)	8.99790E+01	5.95174E+00	1.34650E-04	5.99751E+00
16)	1.47328E+02	5.92953E+00	1.46822E-04	5.99637E+00
0)	OH-			
1)	9.95011E-10			
2)	7.56894E-10			
3)	5.72213E-10			
4)	3.75209E-10			
5)	2.37467E-10			
6)	1.63408E-10			
7)	1.21264E-10			
8)	9.36659E-11			
9)	7.38291E-11			
10)	5.88434E-11			
11)	4.72634E-11			
12)	3.82895E-11			
13)	3.14644E-11			
14)	2.65307E-11			
15)	2.32879E-11			
16)	2.14222E-11			
0)	Th++++	Th(OH)4(aq)		
1)	3.10808E-09	1.31972E-09		
2)	9.28248E-09	1.31972E-09		
3)	2.84166E-08	1.31971E-09		
4)	1.53713E-07	1.31971E-09		

Figure 6.3.4 Edited Listing of the Output File FMT_THO2_6MNACL_QB0204.TITRATE
(Page 2 of 2)

5)	9.58060E-07	1.31971E-09
6)	4.27289E-06	1.31971E-09
7)	1.40902E-05	1.31971E-09
8)	3.95926E-05	1.31969E-09
9)	1.02626E-04	1.31965E-09
10)	2.54639E-04	1.31956E-09
11)	6.13646E-04	1.31935E-09
12)	1.43444E-03	1.31886E-09
13)	3.19252E-03	1.31782E-09
14)	6.49439E-03	1.31588E-09
15)	1.14086E-02	1.31302E-09
16)	1.66743E-02	1.30998E-09

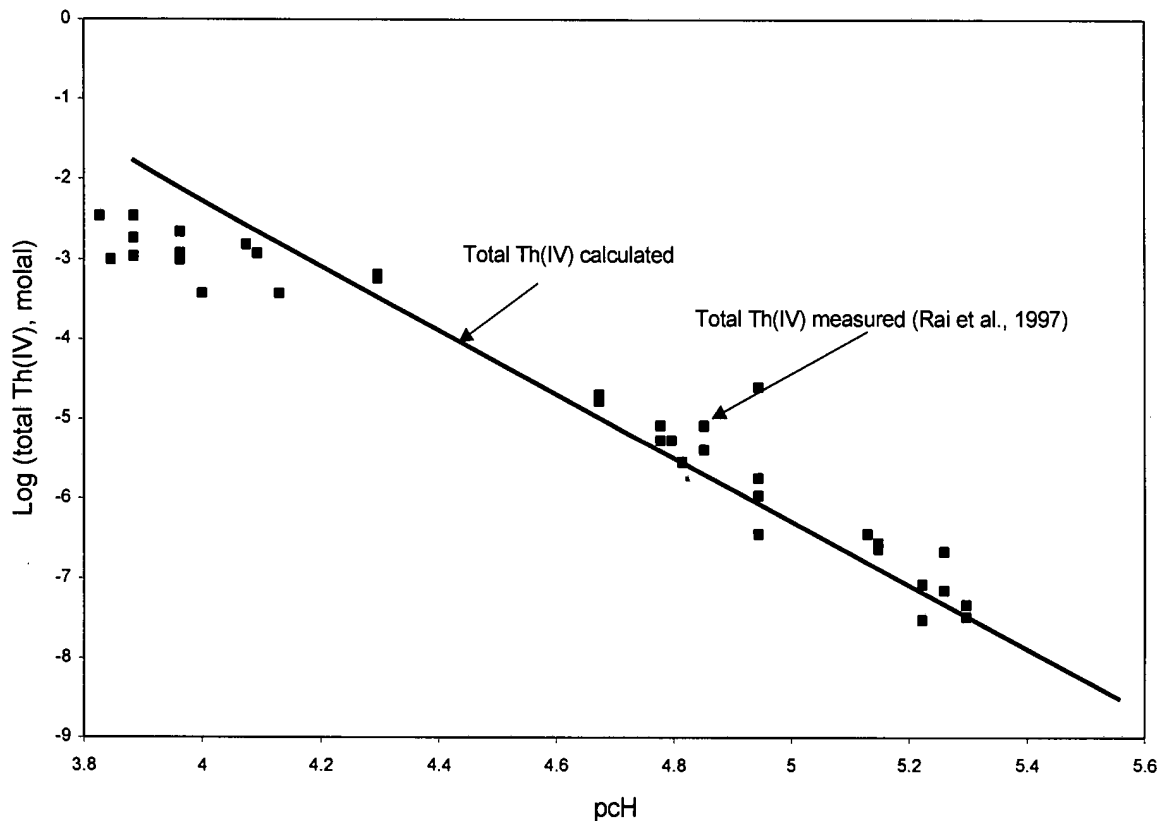
0)	IonicStrength	Titrvol,ml	pH	pmH
1)	5.99998E+00	0.000000000E+00	4.852	5.504
2)	5.99998E+00	1.000000000E-02	4.733	5.386
3)	5.99998E+00	2.391360215E-02	4.611	5.264
4)	5.99998E+00	5.718603680E-02	4.428	5.081
5)	5.99998E+00	0.136752413	4.229	4.882
6)	6.00000E+00	0.327024280	4.067	4.720
7)	6.00006E+00	0.782032854	3.938	4.590
8)	6.00021E+00	1.87012225	3.825	4.478
9)	6.00057E+00	4.47213595	3.722	4.375
10)	6.00145E+00	10.6944880	3.623	4.276
11)	6.00353E+00	25.5743731	3.528	4.181
12)	6.00828E+00	61.1575384	3.436	4.089
13)	6.01844E+00	146.249704	3.350	4.004
14)	6.03754E+00	349.735724	3.275	3.929
15)	6.06596E+00	836.344097	3.216	3.871
16)	6.09642E+00	2000.00000	3.177	3.833

6.3.4 Evaluation

The calculated ThO_2 (am) solubility was to be graphically compared with the experimental data from Rai et al. (1997). The model prediction was expected to follow the general trend of the experimental data and the deviation of the model prediction from the experimental data was to be less than half a logarithmic unit.

Figure 6.3.3 shows the the nonzero concentrations calculated by FMT. Figure 6.3.4 shows the nonzero titration results from FMT. Figure 6.3.5 graphically compares the total Th(IV) calculated by FMT with the experimental measurements of Rai et al. (1997). It can be seen that the deviation of the model prediction from most experimental data points was less that half a logarithmic unit. Considering scattering of the experimental data, the acceptance criteria is considered to have been met.

Figure 6.3.5 Graphical Comparison of the Total Th(IV) Calculated by FMT and the Experimental Measurements of Rai et al (1997)



6.4 Test Case #4: Solubility of $\text{NaAm}(\text{CO}_3)_2 \cdot 6\text{H}_2\text{O}$ in Na_2CO_3 and NaHCO_3 Solutions

6.4.1 Test Objectives

Using the “titration” modes of logarithmic increments and linear increments, respectively, FMT calculates the solubility of $\text{NaAm}(\text{CO}_3)_2 \cdot 6\text{H}_2\text{O}$ in Na_2CO_3 and NaHCO_3 solutions as a function of total carbonate concentration. This test cases addresses requirements R.2, R.4, and R.7.

6.4.2 Test Procedures

This test case was run using the script FMT_TEST_QB0204.COM. This command file is shown in **Figure 6.0.2**.

6.4.3 Input/Output Files

The following is a list of all files associated with Test Case #4:

Command file:

FMT_TEST_QB0204.COM

Input files:

FMT_AM_NA2CO3.IN	(See Figure 6.4.1)
FMT_AM_NA2CO3.INGUESS	(See Figure 6.4.2)
FMT_AM_NAHCO3.IN	(See Figure 6.4.3)
FMT_AM_NAHCO3.INGUESS	(See Figure 6.4.4)

Output files:

FMT_AM_NA2CO3_QB0204.OUT	(See Figure 6.4.5)
FMT_AM_NA2CO3_QB0204.TITRATE	(See Figure 6.4.6)
FMT_AM_NAHCO3_QB0204.OUT	(See Figure 6.4.7)
FMT_AM_NAHCO3_QB0204.TITRATE	(See Figure 6.4.8)

Figure 6.4.1 Listing of the Input File FMT_AM_NA2CO3.IN
(Page 1 of 2)

```
'Benchmark: Solubility of NaAm(CO3)2.6H2O(s) versus Na2CO3'  
'CHEMFILE'  
'TITRATE' 'EXPLICIT'  
'DISABLE_SPECIES' 0  
'nSET_FC02' 0.0  
'nSET_PH' 0.0
```

```
'nMOLES' 'nEXACT' H2O Saturated with Natron  
3.11031293E+02 Hydrogen  
1.93591147E+02 Oxygen  
2.53836668E+01 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
1.26918334E+01 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
3.55271368E-15 Charge:EL
```

```
'nMOLES' 'nEXACT' H2O Saturated with NaAm(CO3)2.6H2O(s)  
1.31094441E+03 Hydrogen  
1.25521687E+03 Oxygen  
1.00000000E+02 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
1.99927048E+02 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
9.99270479E+01 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
-1.98301441E-17 Charge:EL
```

```
20 2.25d3 0.0025d0 1.800001d5 'NDXVARIABLE'  
'nDIFFUS',  
'CONVEC',
```

Figure 6.4.1 Listing of the Input File FMT_AM_NA2CO3.IN
(Page 2 of 2)

```
'nSSDIFF',  
'nRESTART',  
'nPUSHPULL', 'nMULTINJ',  
  
20 1 20 'nLOTS' 10  
'nTGRAD' 'LINEAR'  
'FRAC FLO', 'nTWO PHASE', 'nMASS TR',  
3  
0.1d0 0.2d0 0.3d0  
1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF', 'LHSFDIF', vfrd dfrc FPOR mpor dmxt  
'nMOLES' 'nEXACT' Plain old pure H2O  
1.11017364E+02 Hydrogen  
5.55086820E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E-00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL  
  
1.d-12 1.d-20 (fracture, matrix permeabilities)  
'VPOROS', 'FRFLASH', (NOFLASH or FRFLASH, default is all flash)  
'VAR_AQ_RHO' 1074.9d0  
'nNO X DIFF',  
'UNIFORM', 0  
  
'TITRATE', 'LOG10', 0.03, 20.0, 'INJSOLIDS'
```

Figure 6.4.2 Listing of the Input File FMT_AM_NA2CO3.INGUESS

(This file is necessary but is intentionally blank for this test case.)

Figure 6.4.3 Listing of the Input File FMT_AM_NAHCO3.IN
(Page 1 of 2)

```
'Benchmark: Solubility of NaAm(CO3)2.6H2O(s) versus NaHCO3'  
'CHEMFILE'  
'TITRATE' 'EXPLICIT'  
'DISABLE_SPECIES' 0  
'nSET_FC02' 0.0  
'nSET_PH' 0.0
```

```
'nMOLES' 'nEXACT' H2O Saturated with Nahcolite  
1.22202086E+02 Hydrogen  
8.91540089E+01 Oxygen  
1.12211864E+01 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
1.12211864E+01 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
3.40005801E-16 Charge:EL
```

```
'nMOLES' 'nEXACT' H2O Saturated with NaAm(CO3)2.6H2O(s)  
1.31094441E+03 Hydrogen  
1.25521687E+03 Oxygen  
1.00000000E+02 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
1.99927048E+02 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
9.99270479E+01 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
-1.98301441E-17 Charge:EL
```

```
40 2.25d3 0.0025d0 1.800001d5 'NDXVARIABLE'  
'nDIFFUS',  
'CONVEC',
```

Figure 6.4.3 Listing of the Input File FMT_AM_NAHCO3.IN
(Page 2 of 2)

```
'nSSDIFF',
'nRESTART',
'nPUSHPULL', 'nMULTINJ',

20 1 20 'nLOTS' 10
'nTGRAD' 'LINEAR'
'FRAC_FLO', 'nTWO PHASE', 'nMASS TR',
3

0.1d0 0.2d0 0.3d0
1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF', 'LHSFDIF', vfrc dfrc FPOR mpor dmxt
'nMOLES' 'nEXACT' Plain old pure H2O
1.11017364E+02 Hydrogen
5.55086820E+01 Oxygen
0.00000000E+00 Sodium
0.00000000E+00 Potassium
0.00000000E+00 Magnesium
0.00000000E+00 Calcium
0.00000000E-00 Chlorine
0.00000000E+00 Sulfur
0.00000000E+00 Carbon
0.00000000E+00 PosIon:EL
0.00000000E+00 NegIon:EL
0.00000000E+00 Oxalate:EL
0.00000000E+00 Boron
0.00000000E+00 Bromine
0.00000000E+00 Acetate:EL
0.00000000E+00 Th(IV)
0.00000000E+00 Am(III)
0.00000000E+00 U(VI)
0.00000000E+00 Np(V)
0.00000000E+00 ClO4:EL
0.00000000E+00 Phosphorus
0.00000000E+00 U(IV)
0.00000000E+00 Lactate:EL
0.00000000E+00 EDTA:EL
0.00000000E+00 Citrate:EL
0.00000000E+00 Electron:E
0.00000000E+00 Charge:EL

1.d-12 1.d-20 (fracture, matrix permeabilities)
'VPOROS', 'FRFLASH', (NOFLASH or FRFLASH, default is all flash)
'VAR_AQ_RHO' 1074.9d0
'nNO X DIFF',
'UNIFORM', 0

'TITRATE', 'LINEAR', 0.121, 4.7, 'INJSOLIDS'
```

Figure 6.4.4 Listing of the Input File FMT_AM_NAHCO3.INGUESS

(This file is necessary but is intentionally blank for this test case.)

Figure 6.4.5 Edited Listing of the Output File FMT_AM_NA2CO3_QB0204.OUT
(Page 1 of 5)

INPUT file name is:WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AM_NA2CO3.IN;1
 INGUESS file name is:WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AM_NA2CO3.INGUESS;1
 OUTPUT file name is:WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AM_NA2CO3_QB0204.OUT;1
 CHEMDAT file name is:WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
 Temperature is Hard Coded as 298.15K
 Benchmark: Solubility of NaAm(CO3)2.6H2O(s) versus Na2CO3 FMT V2.4
 FMT_ph_970407.chemdat
 Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5== by analogy

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.72900E-01	9.00626E-01	1.032	5.55087E+01	5.03842E+01	9.07682E+05
Na2CO3.10H2O	Na2CO3	1.00000E+01	1.00000E+00	1.000	1.00000E+01	9.07682E+00	2.59725E+06
Na+	Na+	5.38367E+00	2.88867E+00	0.5366	5.38367E+00	4.88666E+00	1.12343E+05
OH-	OH-	6.96498E-03	6.32897E-03	0.9087	6.96498E-03	6.32199E-03	1.07520E+02
CO3=	CO3=	2.68487E+00	5.11017E-02	1.9033E-02	2.68487E+00	2.43701E+00	1.46243E+05
HCO3-	HCO3-	6.96498E-03	6.0043E-03	0.2298	6.96498E-03	6.32199E-03	3.85749E+02
CO2(aq)	CO2(aq)	1.88828E-09	5.54224E-09	2.935	1.88828E-09	1.71396E-09	7.54308E-05
H+	H+	3.69891E-12	1.43401E-12	0.3877	3.69891E-12	3.35744E-12	3.38396E-09
							5.94E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.97357E-01	9.97557E-01	1.000	5.58797E+01	5.54390E+01	9.98744E+05
NaAm(CO3)2.6H2O(c)	NaAm(CO3)2.6H2O(c)	9.92624E+01	1.00000E+00	1.000	9.92624E+01	9.91378E+01	4.89839E+07
Na+	Na+	7.35404E-02	5.70177E-02	0.7753	7.40320E-02	7.34481E-02	1.68855E+03
HCO3-	HCO3-	7.17417E-02	5.54720E-02	0.7732	7.22213E-02	7.16516E-02	4.37197E+03
CO2(aq)	CO2(aq)	9.00252E-04	9.13591E-04	1.015	9.06270E-04	8.99121E-04	3.95702E+01
CO3=	CO3=	8.98457E-04	3.36242E-04	0.3742	9.04463E-04	8.97329E-04	5.38480E+01
OH-	OH-	1.66896E-06	1.33078E-06	0.7974	1.68012E-06	1.66687E-06	2.83489E-02
Am(CO3)3=	Am(CO3)3=	3.73302E-08	3.61342E-09	9.6796E-02	3.75797E-08	3.72833E-08	1.57719E-02
Am(CO3)2-	Am(CO3)2-	1.83893E-08	1.41023E-08	0.7669	1.85122E-08	1.83662E-08	6.66727E-03
H+	H+	9.78996E-09	7.55393E-09	0.7716	9.85540E-09	9.77766E-09	9.85491E-06
AmCO3+	AmCO3+	1.03314E-09	7.92958E-10	0.7675	1.04004E-09	1.03184E-09	3.12656E-04
Am+++	Am+++	1.07521E-12	6.40206E-14	5.9542E-02	1.08240E-12	1.07386E-12	6.60949E-07
Am(OH)3(aq)	(1e-9m minimum)	2.39019E-14	2.39019E-14	1.000	2.40617E-14	2.38719E-14	7.01886E-09
AmOH++	(after_Cm(III))	7.24537E-15	2.34540E-15	0.3237	7.29380E-15	7.23627E-15	1.88148E-09
Am(OH)2+	(after_Cm(III))	2.94848E-15	2.26304E-15	0.7675	2.96819E-15	2.94478E-15	8.15747E-10
AmOHC03(c)	AmOHC03(c)	1.07268E-03	1.00000E+00	1.000	1.07985E-03	1.07134E-03	3.42845E+02
							-5.79E-08
							1.35E-07
							1.17E-07
							1.94E-08
							-1.39E-08
							-9.70E-08
							-2.43E-07
							1.98E-07
							-8.75E-08
							5.85E-08
							-9.39E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.97357E-01	9.97557E-01	1.000	2.17475E+00	5.54390E+01	9.98744E+05
NaAm(CO3)2.6H2O(c)	NaAm(CO3)2.6H2O(c)	9.92624E+01	1.00000E+00	1.000	3.88896E+00	9.91378E+01	4.89839E+07
Na+	Na+	7.35404E-02	5.70177E-02	0.7753	2.88121E-03	7.34481E-02	1.68855E+03
HCO3-	HCO3-	7.17417E-02	5.54720E-02	0.7732	2.81074E-03	7.16516E-02	4.37197E+03
CO2(aq)	CO2(aq)	9.00252E-04	9.13591E-04	1.015	3.52705E-05	8.99121E-04	3.95702E+01
AmOHC03(c)	AmOHC03(c)	1.07268E-03	1.00000E+00	1.000	4.20261E-05	1.07134E-03	3.42845E+02
CO3=	CO3=	8.98457E-04	3.36242E-04	0.3742	3.52002E-05	8.97329E-04	5.38480E+01
OH-	OH-	1.66896E-06	1.33078E-06	0.7974	6.53875E-08	1.66687E-06	2.83489E-02
Am(CO3)3=	Am(CO3)3=	3.73302E-08	3.61342E-09	9.6796E-02	1.46254E-09	3.72833E-08	1.57719E-02
Am(CO3)2-	Am(CO3)2-	1.83893E-08	1.41023E-08	0.7669	7.20466E-10	1.83662E-08	6.66727E-03
H+	H+	9.78996E-09	7.55393E-09	0.7716	3.83556E-10	9.77766E-09	9.85491E-06
AmCO3+	AmCO3+	1.03314E-09	7.92958E-10	0.7675	4.04767E-11	1.03184E-09	3.12656E-04
Am+++	Am+++	1.07521E-12	6.40206E-14	5.9542E-02	4.21253E-14	1.07386E-12	2.60949E-07
Am(OH)3(aq)	(1e-9m minimum)	2.39019E-14	2.39019E-14	1.000	9.35842E-16	2.38719E-14	7.01886E-09
AmOH++	(after_Cm(III))	7.24537E-15	2.34540E-15	0.3237	2.83863E-16	7.23627E-15	1.88148E-09
Am(OH)2+	(after_Cm(III))	2.94848E-15	2.26304E-15	0.7675	1.15517E-16	2.94478E-15	8.15747E-10
							6.98E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.96927E-01	9.97211E-01	1.000	2.17874E+00	5.54221E+01	9.98441E+05
NaAm(CO3)2.6H2O(c)	NaAm(CO3)2.6H2O(c)	9.90816E+01	1.00000E+00	1.000	3.88900E+00	9.89271E+01	4.88798E+07
Na+	Na+	8.99454E-02	6.84825E-02	0.7614	3.53040E-03	8.98052E-02	2.06460E+03
HCO3-	HCO3-	7.21629E-02	5.36761E-02	0.7438	2.83243E-03	7.20504E-02	4.39631E+03
CO3=	CO3=	8.88279E-03	3.00565E-03	0.3384	3.48654E-04	8.86894E-03	5.32218E+02
CO2(aq)	CO2(aq)	9.40193E-05	9.57260E-05	1.018	3.69030E-06	9.38727E-05	4.13132E+00
OH-	OH-	1.58994E-05	1.22895E-05	0.7730	6.24061E-07	1.58747E-05	2.69885E-01
Am(CO3)3=	Am(CO3)3=	3.38344E-07	2.69488E-08	7.9649E-02	1.32802E-08	3.37816E-07	1.42906E-01
Am(CO3)2-	Am(CO3)2-	1.59643E-08	1.17659E-08	0.7370	6.26604E-10	1.59394E-08	5.78628E-03
H+	H+	1.09416E-09	8.17699E-10	0.7473	4.29461E-11	1.09245E-09	1.10108E-06
AmCO3+	AmCO3+	9.96774E-11	7.40114E-11	0.7425	3.91238E-12	9.95220E-11	3.01561E-05
Am(OH)3(aq)	(1e-9m minimum)	1.96554E-13	1.96554E-13	1.000	7.71482E-15	1.96247E-13	5.77009E-08
Am+++	Am+++	1.56248E-14	6.68469E-16	4.2783E-02	6.13281E-16	1.56004E-14	3.79091E-09
Am(OH)2+	(after_Cm(III))	2.71400E-15	2.01517E-15	0.7425	1.06526E-16	2.70976E-15	7.50644E-10
AmOH++	(after_Cm(III))	8.02173E-16	2.26156E-16	0.2819	3.14857E-17	8.00922E-16	2.08246E-10
							1.16E-10
							-1.06E-11
							-9.10E-11
							5.84E-12
							1.01E-10
							9.53E-11
							-1.24E-10
							-2.74E-07
							-2.28E-11
							7.42E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.96724E-01	9.97048E-01	1.000	2.18058E+00	5.54142E+01	9.98297E+05
NaAm(CO3)2.6H2O(c)	NaAm(CO3)2.6H2O(c)	9.89979E+01	1.00000E+00	1.000	3.88900E+00	9.88293E+01	4.88315E+07
Na+	Na+	9.75254E-02	7.37278E-02	0.7560	3.83115E-03	9.73594E-02	2.23827E+03
HCO3-	HCO3-	7.21634E-02	5.28212E-02	0.7320	2.83484E-03	7.20405E-02	4.39570E+03

Figure 6.4.5 Edited Listing of the Output File FMT_AM_NA2CO3_QB0204.OUT
(Page 2 of 5)

CO3=	CO3=	1.26691E-02	4.11159E-03	0.3245	4.97689E-04	1.26475E-02	7.58968E+02	
CO2 (aq)	CO2 (aq)	6.64681E-05	6.77773E-05	1.020	2.61111E-06	6.63549E-05	2.92027E+00	8.85E-11
OH-	OH-	2.23778E-05	1.70807E-05	0.7633	8.79083E-07	2.23397E-05	3.79938E-01	-7.67E-11
Am(CO3) 3=-	Am(CO3) 3=-	4.67003E-07	3.42756E-08	7.3395E-02	1.83456E-08	4.66207E-07	1.97219E-01	-6.26E-11
Am(CO3) 2=-	Am(CO3) 2=-	1.50896E-08	1.09395E-08	0.7250	5.92776E-10	1.50639E-08	5.46849E-03	5.23E-12
H+	H+	7.97618E-10	5.88234E-10	0.7375	3.13333E-11	7.96260E-10	8.02550E-07	7.28E-11
AmCO3+	AmCO3+	6.86904E-11	5.03039E-11	0.7323	2.69841E-12	6.85734E-11	2.07784E-05	6.63E-11
Am(OH) 3 (aq)	(1e-9m_minimum)	2.62199E-13	2.62199E-13	1.000	1.03001E-14	2.61753E-13	7.69610E-08	-9.55E-11
Am+++	Am+++	8.91945E-13	3.32134E-16	3.7237E-02	3.50389E-16	8.90426E-15	2.16374E-09	-3.47E-08
Am(OH) 2+	(after_Cm(III))	2.64109E-15	1.93414E-15	0.7323	1.03752E-16	2.63659E-15	7.30374E-10	-2.27E-11
AmOH++	(after_Cm(III))	5.86883E-16	1.56175E-16	0.2661	2.30549E-17	5.85884E-16	1.52334E-10	4.59E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.96433E-01	9.96816E-01	1.000	2.18323E+00	5.54027E+01	9.98092E+05	
NaAm(CO3) 2.6H2O(c)		9.88781E+01	1.00000E+00	1.000	3.88900E+00	9.86894E+01	4.87624E+07	
Na+	Na+	1.08381E-01	8.11864E-02	0.7491	4.26277E-03	1.08174E-01	2.48690E+03	
HCO3-	HCO3-	7.21240E-02	5.16811E-02	0.7166	2.83673E-03	7.19864E-02	4.39240E+03	
CO3=	CO3=	1.81119E-02	5.56181E-03	0.3071	7.12363E-04	1.80773E-02	1.08480E+03	
CO2 (aq)	CO2 (aq)	4.69474E-05	4.79761E-05	1.022	1.84650E-06	4.68578E-05	2.06220E+00	6.87E-11
OH-	OH-	3.14417E-05	2.36096E-05	0.7509	1.23664E-06	3.13817E-05	5.33718E-01	-5.67E-11
Am(CO3) 3=-	Am(CO3) 3=-	6.40835E-07	4.21645E-08	6.5796E-02	2.52048E-08	6.39612E-07	2.70574E-01	-4.32E-11
Am(CO3) 2=-	Am(CO3) 2=-	1.40257E-08	9.94838E-09	0.7093	5.51648E-10	1.39989E-08	5.08187E-03	4.75E-12
H+	H+	5.87153E-10	4.25468E-10	0.7246	2.30935E-11	5.86032E-10	5.90662E-07	5.31E-11
AmCO3+	AmCO3+	4.70352E-11	3.38181E-11	0.7190	1.84996E-12	4.69455E-11	1.42249E-05	4.61E-11
Am(OH) 3 (aq)	(1e-9m_minimum)	3.44128E-13	3.44128E-13	1.000	1.35350E-14	3.43471E-13	1.00988E-07	-7.59E-11
Am+++	Am+++	5.33803E-15	1.65065E-16	3.0922E-02	2.09952E-16	5.32785E-15	1.29467E-09	-7.10E-08
Am(OH) 2+	(after_Cm(III))	2.55428E-15	1.83651E-15	0.7190	1.00463E-16	2.54940E-15	7.06222E-10	-2.28E-11
AmOH++	(after_Cm(III))	4.35432E-16	1.07284E-16	0.2464	1.71261E-17	4.34601E-16	1.12999E-10	2.65E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.96018E-01	9.96486E-01	1.000	2.18702E+00	5.53864E+01	9.97798E+05	
NaAm(CO3) 2.6H2O(c)		9.87065E+01	1.00000E+00	1.000	3.88900E+00	9.84892E+01	4.86634E+07	
Na+	Na+	1.23914E-01	9.17611E-02	0.7405	4.88218E-03	1.23641E-01	2.84249E+03	
HCO3-	HCO3-	7.20389E-02	5.10275E-02	0.6971	2.83830E-03	7.18803E-02	4.38592E+03	
CO3=	CO3=	2.59144E-02	7.40870E-03	0.2859	1.02102E-03	2.58574E-02	1.55168E+03	
OH-	OH-	4.39885E-05	3.23554E-05	0.7355	1.73313E-06	4.38916E-05	7.46478E-01	-4.43E-11
CO2 (aq)	CO2 (aq)	3.31839E-05	3.40166E-05	1.025	1.30743E-06	3.31108E-05	1.45720E+00	5.45E-11
Am(CO3) 3=-	Am(CO3) 3=-	8.72970E-07	4.97920E-08	5.7037E-02	3.43947E-08	8.71048E-07	3.68477E-01	-3.02E-11
Am(CO3) 2=-	Am(CO3) 2=-	1.27915E-08	8.81940E-09	0.6895	5.03980E-10	1.27633E-08	4.63332E-03	4.03E-12
H+	H+	4.38177E-10	3.10359E-10	0.7083	1.72640E-11	4.37212E-10	4.40666E-07	4.07E-11
AmCO3+	AmCO3+	3.20605E-11	2.25066E-11	0.7020	1.26317E-12	3.19899E-11	9.63924E-06	3.26E-11
Am(OH) 3 (aq)	(1e-9m_minimum)	4.42517E-13	4.42517E-13	1.000	1.74350E-14	4.41543E-13	1.29823E-07	-6.48E-11
Am+++	Am+++	3.40276E-15	8.24689E-17	2.4236E-02	1.34067E-16	3.39527E-15	8.25050E-10	-2.00E-08
Am(OH) 2+	(after_Cm(III))	2.45475E-15	1.72324E-15	0.7020	9.67160E-17	2.44934E-15	6.78503E-10	-2.42E-11
AmOH++	(after_Cm(III))	3.29661E-16	7.34564E-17	0.2228	1.29885E-17	3.28935E-16	8.55256E-11	1.31E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95424E-01	9.96019E-01	1.001	2.19246E+00	5.53632E+01	9.97379E+05	
NaAm(CO3) 2.6H2O(c)		9.84614E+01	1.00000E+00	1.000	3.88900E+00	9.82033E+01	4.85222E+07	
Na+	Na+	1.46112E-01	1.06700E-01	0.7303	5.77109E-03	1.45729E-01	3.35028E+03	
HCO3-	HCO3-	7.18965E-02	4.84031E-02	0.6732	2.83975E-03	7.17080E-02	4.37542E+03	
CO3=	CO3=	3.70755E-02	9.6848E-03	0.2613	1.46440E-03	3.69783E-02	2.21904E+03	
OH-	OH-	6.11657E-05	4.38682E-05	0.7172	2.41590E-06	6.10053E-05	1.03754E+00	-3.31E-11
CO2 (aq)	CO2 (aq)	2.34863E-05	2.41828E-05	1.030	9.27656E-07	2.34248E-05	1.03092E+00	4.53E-11
Am(CO3) 3=-	Am(CO3) 3=-	1.18108E-06	5.61431E-08	4.7535E-02	4.66500E-08	1.17799E-06	4.98321E-01	-2.05E-11
Am(CO3) 2=-	Am(CO3) 2=-	1.14348E-08	7.60593E-09	0.6652	4.51649E-10	1.14049E-08	4.14017E-03	3.40E-12
H+	H+	3.32468E-10	2.28801E-10	0.6882	1.31317E-11	3.31597E-10	3.34216E-07	3.03E-11
AmCO3+	AmCO3+	2.18002E-11	1.48457E-11	0.6810	8.61058E-13	2.17431E-11	6.58834E-06	2.20E-11
Am(OH) 3 (aq)	(1e-9m_minimum)	5.56419E-13	5.56419E-13	1.000	2.19773E-14	5.54961E-13	1.63171E-07	-5.34E-11
Am(OH) 2+	(after_Cm(III))	2.34681E-15	1.59815E-15	0.6810	9.26934E-17	2.34065E-15	6.48395E-10	-2.32E-11
Am+++	Am+++	2.34605E-15	4.16060E-17	1.7734E-02	9.26637E-17	2.33990E-15	5.68597E-10	-1.16E-09
AmOH++	(after_Cm(III))	2.56332E-16	5.02455E-17	0.1960	1.01245E-17	2.55660E-16	6.64734E-11	4.07E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.94579E-01	9.95361E-01	1.001	2.20028E+00	5.53300E+01	9.96781E+05	
NaAm(CO3) 2.6H2O(c)		9.81117E+01	1.00000E+00	1.000	3.88900E+00	9.77959E+01	4.83209E+07	
Na+	Na+	1.77776E-01	1.27714E-01	0.7184	7.04678E-03	1.77204E-01	4.07388E+03	
HCO3-	HCO3-	7.16781E-02	4.62271E-02	0.6449	2.84121E-03	7.14474E-02	4.35951E+03	
CO3=	CO3=	5.30045E-02	1.23998E-02	0.2339	2.10102E-03	5.28339E-02	3.17052E+03	
OH-	OH-	8.44063E-05	5.87066E-05	0.6962	3.34573E-06	8.41346E-05	1.43090E+00	-1.70E-09
CO2 (aq)	CO2 (aq)	1.66399E-05	1.72422E-05	1.036	6.59581E-07	1.65863E-05	7.29962E-01	-1.75E-09
Am(CO3) 3=-	Am(CO3) 3=-	1.59116E-06	6.02828E-08	3.7886E-02	6.30713E-08	1.58604E-06	6.70939E-01	5.63E-11
Am(CO3) 2=-	Am(CO3) 2=-	1.00270E-08	6.37973E-09	0.6363	3.97456E-10	9.99474E-09	3.62827E-03	1.82E-11
H+	H+	2.56984E-10	1.70700E-10	0.6642	1.01864E-11	2.56156E-10	2.58180E-07	4.39E-10
AmCO3+	AmCO3+	1.48331E-11	9.72753E-12	0.6558	5.87962E-13	1.47854E-11	4.48010E-06	6.80E-12
Am(OH) 3 (aq)	(1e-9m_minimum)	6.84492E-13	6.84492E-13	1.000	2.71322E-14	6.82289E-13	2.00608E-07	-1.32E-09
Am(OH) 2+	(after_Cm(III))	2.23808E-15	1.46773E-15	0.6558	8.87141E-17	2.23088E-15	6.17985E-10	-8.73E-10
Am+++	Am+++	1.77550E-15	2.12966E-17	1.1995E-02	7.03782E-17	1.76979E-15	4.30059E-10	2.00E-11
AmOH++	(after_Cm(III))	2.06150E-16	3.44500E-17	0.1671	8.17148E-18	2.05487E-16	5.34280E-11	-4.26E-10

Figure 6.4.5 Edited Listing of the Output File FMT_AM_NA2CO3_QB0204.OUT
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.93379E-01	9.94437E-01	1.001	2.21149E+00	5.52829E+01	9.95932E+05
NaAm(CO3)2.6H2O(c)		9.76142E+01	1.00000E+00	1.000	3.88900E+00	9.72171E+01	4.80349E+07
Na+	Na+	2.22827E-01	1.57113E-01	0.7051	8.87753E-03	2.21920E-01	5.10190E+03
CO3=	CO3=	7.56746E-02	1.55134E-02	0.2050	3.01491E-03	7.53668E-02	4.52270E+03
HCO3-	HCO3-	7.13545E-02	4.36979E-02	0.6124	2.84285E-03	7.10654E-02	4.33620E+03
OH-	OH-	1.15444E-04	7.76985E-05	0.6730	4.59934E-06	1.14974E-04	1.95540E+00
CO2(aq)	CO2(aq)	1.17889E-05	1.23262E-05	1.046	4.69678E-07	1.17410E-05	5.16719E-01
Am(CO3)3=-	Am(CO3)3=-	2.14541E-06	6.16500E-08	2.8736E-02	8.54742E-08	2.13668E-06	9.03876E-01
Am(CO3)2-	Am(CO3)2-	8.64846E-09	5.21493E-09	0.6030	3.44559E-10	8.61328E-09	3.12678E-03
H+	H+	2.02570E-10	1.28975E-10	0.6267	4.07051E-12	2.01746E-10	2.03340E-07
AmCO3+	AmCO3+	1.01437E-11	6.35559E-12	0.6266	4.04129E-13	1.01024E-11	3.06112E-06
Am(OH)3(aq)	(1e-9m_minimum)	8.26433E-13	8.26433E-13	1.000	3.29255E-14	8.23072E-13	2.42001E-07
Am(OH)2+	(after_Cm(III))	2.13893E-15	1.34017E-15	0.6266	8.52163E-17	2.13023E-15	5.90106E-10
Am+++	Am+++	1.49587E-15	1.11217E-17	7.4350E-03	5.95962E-17	1.48978E-15	3.62017E-10
AmOH++	(after_Cm(III))	1.72813E-16	2.37890E-17	0.1377	6.88495E-18	1.72110E-16	4.47498E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.91683E-01	9.93150E-01	1.001	2.22759E+00	5.52162E+01	9.94732E+05
NaAm(CO3)2.6H2O(c)		9.69089E+01	1.00000E+00	1.000	3.88900E+00	9.63984E+01	4.76304E+07
Na+	Na+	2.86686E-01	1.97959E-01	0.6905	1.15048E-02	2.85176E-01	6.55612E+03
CO3=	CO3=	1.07816E-01	1.89444E-02	0.1757	4.32672E-03	1.07248E-01	6.43588E+03
HCO3-	HCO3-	7.08885E-02	4.08433E-02	0.5762	2.84479E-03	7.05150E-02	4.30262E+03
OH-	OH-	1.56269E-04	1.01382E-04	0.6488	6.27117E-06	1.55446E-04	2.64372E+00
CO2(aq)	CO2(aq)	8.33757E-06	8.82960E-06	1.059	3.34591E-07	8.29365E-06	3.65002E-01
Am(CO3)3=-	Am(CO3)3=-	2.91833E-06	6.02169E-08	2.0634E-02	1.17114E-07	2.90295E-06	1.22803E+00
Am(CO3)2-	Am(CO3)2-	7.37109E-09	4.17119E-09	0.5659	2.95805E-10	7.33226E-09	2.66174E-03
H+	H+	1.62885E-10	9.87171E-11	0.6061	6.53664E-12	1.62027E-10	1.63307E-07
AmCO3+	AmCO3+	7.01207E-12	4.16288E-12	0.5937	2.81398E-13	6.97513E-12	2.11353E-06
Am(OH)3(aq)	(1e-9m_minimum)	9.84741E-13	9.84741E-13	1.000	3.95181E-14	9.79553E-13	2.88010E-07
Am(OH)2+	(after_Cm(III))	2.06146E-15	1.22384E-15	0.5937	8.27275E-17	2.05060E-15	5.68047E-10
Am+++	Am+++	1.42149E-15	5.96534E-18	4.1965E-03	5.70450E-17	1.41400E-15	3.43602E-10
AmOH++	(after_Cm(III))	1.52262E-16	1.66491E-17	0.1093	6.11034E-18	1.51460E-16	3.93806E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.89301E-01	9.91375E-01	1.002	2.25069E+00	5.51225E+01	9.93044E+05
NaAm(CO3)2.6H2O(c)		9.59144E+01	1.00000E+00	1.000	3.88900E+00	9.52472E+01	4.70616E+07
Na+	Na+	3.76735E-01	2.54192E-01	0.6747	1.52753E-02	3.74114E-01	8.60080E+03
CO3=	CO3=	1.53147E-01	2.25572E-02	0.1473	6.20958E-03	1.52082E-01	9.12630E+03
HCO3-	HCO3-	7.02200E-02	3.77097E-02	0.5370	2.84718E-03	6.97316E-02	4.25482E+03
OH-	OH-	2.08970E-04	1.30515E-04	0.6246	8.47302E-06	2.07516E-04	3.52929E+00
CO2(aq)	CO2(aq)	5.87291E-06	6.33251E-06	1.078	2.38126E-07	5.83205E-06	2.56667E-01
Am(CO3)3=-	Am(CO3)3=-	4.05012E-06	5.64413E-08	1.3936E-02	1.64218E-07	4.02194E-06	1.70139E+00
Am(CO3)2-	Am(CO3)2-	6.24537E-09	3.28348E-09	0.5257	2.53228E-10	6.20193E-09	2.25141E-03
H+	H+	1.33550E-10	7.65454E-11	0.5732	5.41501E-12	1.32621E-10	1.33669E-07
AmCO3+	AmCO3+	4.93366E-12	2.75209E-12	0.5578	2.00043E-13	4.89934E-12	1.48454E-06
Am(OH)3(aq)	(1e-9m_minimum)	1.16648E-12	1.16648E-12	1.000	4.72966E-14	1.15836E-12	3.40584E-07
Am(OH)2+	(after_Cm(III))	2.01877E-15	1.12611E-15	0.5578	8.18541E-17	2.00473E-15	5.55338E-10
Am+++	Am+++	1.54132E-15	3.31207E-18	2.1489E-03	6.24952E-17	1.53060E-15	3.71935E-10
AmOH++	(after_Cm(III))	1.42203E-16	1.19001E-17	8.3684E-02	5.76586E-18	1.41214E-16	3.67167E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.85986E-01	9.88959E-01	1.003	2.28384E+00	5.49919E+01	9.90690E+05
NaAm(CO3)2.6H2O(c)		9.45222E+01	1.00000E+00	1.000	3.88900E+00	9.36423E+01	4.62686E+07
Na+	Na+	5.02782E-01	3.30677E-01	0.6577	2.06864E-02	4.98102E-01	1.14512E+04
CO3=	CO3=	2.16608E-01	2.61671E-02	0.1208	8.91206E-03	2.14591E-01	1.28775E+04
HCO3-	HCO3-	6.92736E-02	3.43594E-02	0.4960	2.85018E-03	6.86287E-02	4.18753E+03
OH-	OH-	2.75373E-04	1.65759E-04	0.6019	1.13299E-05	2.72810E-04	4.63976E+00
Am(CO3)3=-	Am(CO3)3=-	5.81837E-06	5.10723E-08	8.7778E-03	2.39389E-07	5.76420E-06	2.43842E+00
CO2(aq)	CO2(aq)	4.10845E-06	4.54307E-06	1.106	1.69037E-07	4.07020E-06	1.79129E-01
Am(CO3)2-	Am(CO3)2-	5.29600E-09	2.56125E-09	0.4836	2.17897E-10	5.24669E-09	1.90465E-03
H+	H+	1.11528E-10	6.01229E-11	0.5391	4.58867E-12	1.10489E-10	1.11362E-07
AmCO3+	AmCO3+	3.55937E-12	1.85058E-12	0.5199	1.46446E-13	3.52623E-12	1.06848E-06
Am(OH)3(aq)	(1e-9m_minimum)	1.38518E-12	1.38518E-12	1.000	5.69916E-14	1.37229E-12	4.03483E-07
Am(OH)2+	(after_Cm(III))	2.02515E-15	1.05291E-15	0.5199	8.33221E-17	2.00629E-15	5.55773E-10
Am+++	Am+++	1.92359E-15	1.91988E-18	9.9807E-04	7.91435E-17	1.90568E-15	4.63080E-10
AmOH++	(after_Cm(III))	1.41872E-16	8.76082E-18	6.1752E-02	5.83713E-18	1.40551E-16	3.65442E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.81431E-01	9.85721E-01	1.004	2.33141E+00	5.48120E+01	9.87449E+05
NaAm(CO3)2.6H2O(c)		9.25935E+01	1.00000E+00	1.000	3.88900E+00	9.14313E+01	4.51762E+07
Na+	Na+	6.77411E-01	4.43084E-01	0.6393	2.84518E-02	6.68909E-01	1.53781E+04
CO3=	CO3=	3.04539E-01	2.95624E-02	9.7072E-02	1.27909E-02	3.00717E-01	1.80458E+04
HCO3-	HCO3-	6.79492E-02	3.08698E-02	0.4543	2.85392E-03	6.70964E-02	4.09403E+03
OH-	OH-	3.56497E-04	2.07753E-04	0.5828	1.49732E-05	3.52023E-04	5.98696E+00
Am(CO3)3=-	Am(CO3)3=-	8.79928E-06	4.49311E-08	5.1062E-03	3.69577E-07	8.68884E-06	3.67562E+00
CO2(aq)	CO2(aq)	2.84400E-06	3.25663E-06	1.145	1.19450E-07	2.80830E-06	1.23593E-01
Am(CO3)2-	Am(CO3)2-	4.52512E-09	1.99448E-09	0.4408	1.90059E-10	4.46832E-09	1.62208E-03
H+	H+	9.46502E-11	4.78130E-11	0.5052	3.97538E-12	9.34622E-11	9.42006E-08

Figure 6.4.5 Edited Listing of the Output File FMT_AM_NA2CO3_QB0204.OUT
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AmCO3+	AmCO3+	2.65131E-12	1.27557E-12	0.4811	1.11357E-13	2.61804E-12	7.93289E-07	2.47E-14
Am(OH)3(aq)	(1e-9m_minimum)	1.66391E-12	1.66391E-12	1.000	6.98854E-14	1.64302E-12	4.83085E-07	0.00E+00
Am+++	Am+++	2.77209E-15	1.17135E-18	4.2255E-04	1.16430E-16	2.73730E-15	6.65164E-10	-1.90E-09
Am(OH)2+	(after_Cm(III))	2.09750E-15	1.00912E-15	0.4811	8.80966E-17	2.07117E-15	5.73746E-10	-2.47E-14
AmOH++	(after_Cm(III))	1.52035E-16	6.69925E-18	4.4064E-02	6.38560E-18	1.50127E-16	3.90341E-11	1.23E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.75276E-01	9.81463E-01	1.006	2.39968E+00	5.45681E+01	9.83055E+05	
NaAm(CO3)2.6H2O(c)		8.99592E+01	1.00000E+00	1.000	3.88900E+00	8.84348E+01	4.36956E+07	
Na+	Na+	9.15924E-01	5.67556E-01	0.6197	3.95961E-02	9.00404E-01	2.07001E+04	
CO3=	CO3=	4.24653E-01	3.25537E-02	7.6660E-02	1.83581E-02	4.17457E-01	2.50513E+04	
HCO3-	HCO3-	6.61233E-02	2.73301E-02	0.4133	2.85856E-03	6.50028E-02	3.96628E+03	
OH-	OH-	4.51965E-04	2.57290E-04	0.5693	1.95388E-05	4.44307E-04	7.55646E+00	0.00E+00
Am(CO3)3=-	Am(CO3)3=-	1.42468E-05	3.87481E-08	2.7198E-03	6.15900E-07	1.40054E-05	5.92468E+00	0.00E+00
CO2(aq)	CO2(aq)	1.93841E-06	2.32810E-06	1.201	8.37988E-08	1.90556E-06	8.38634E-02	0.00E+00
Am(CO3)2-	Am(CO3)2-	3.91931E-09	1.56197E-09	0.3985	1.69435E-10	3.85290E-09	1.39867E-03	2.47E-14
H+	H+	8.12967E-11	3.84408E-11	0.4728	3.51451E-12	7.99192E-11	8.05050E-08	0.00E+00
AmCO3+	AmCO3+	2.04930E-12	9.07161E-13	0.4427	8.85926E-14	2.01457E-12	6.10434E-07	4.94E-14
Am(OH)3(aq)	(1e-9m_minimum)	2.04113E-12	2.04113E-12	1.000	8.82395E-14	2.00654E-12	5.89686E-07	0.00E+00
Am(OH)2+	(after_Cm(III))	2.25805E-15	9.99567E-16	0.4427	9.76170E-17	2.21979E-15	6.14913E-10	-2.47E-14
AmOH++	(after_Cm(III))	1.75227E-16	5.35821E-18	3.0579E-02	7.57520E-18	1.72258E-16	4.47884E-11	2.47E-14
Am+++	Am+++	4.58589E-15	7.56493E-19	1.6496E-04	1.98251E-16	4.50818E-15	1.09549E-09	-3.44E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.67152E-01	9.75972E-01	1.009	2.49766E+00	5.42447E+01	9.77230E+05	
NaAm(CO3)2.6H2O(c)		8.64302E+01	1.00000E+00	1.000	3.88900E+00	8.44622E+01	4.17327E+07	
Na+	Na+	1.23544E+00	7.40217E-01	0.5992	5.55894E-02	1.20730E+00	2.77556E+04	
CO3=	CO3=	5.85572E-01	3.50456E-02	5.9848E-02	2.63483E-02	5.72239E-01	3.43396E+04	
HCO3-	HCO3-	6.36561E-02	2.38350E-02	0.3744	2.86426E-03	6.22066E-02	3.79567E+03	
OH-	OH-	5.59798E-04	3.15824E-04	0.5642	2.51886E-05	5.47051E-04	9.30387E+00	-1.27E-10
Am(CO3)3=-	Am(CO3)3=-	2.50150E-05	3.30791E-08	1.3224E-03	1.12557E-06	2.44454E-05	1.03411E+01	3.05E-11
CO2(aq)	CO2(aq)	1.29194E-06	1.65406E-06	1.280	5.81319E-08	1.26252E-06	5.55634E-02	-6.81E-10
Am(CO3)2-	Am(CO3)2-	3.45677E-09	1.23863E-09	0.3583	1.55540E-10	3.37806E-09	1.22630E-03	7.93E-12
H+	H+	7.01860E-11	3.11410E-11	0.4437	3.15808E-12	6.85879E-11	6.91297E-07	-2.27E-10
Am(OH)3(aq)	(1e-9m_minimum)	2.58312E-12	2.58312E-12	1.000	1.16230E-13	2.52430E-12	7.42200E-08	6.74E-10
AmCO3+	AmCO3+	1.64616E-12	6.68223E-13	0.4059	7.40701E-14	1.60867E-12	4.87442E-07	-1.97E-13
Am+++	Am+++	8.54730E-15	5.17618E-19	6.0559E-05	3.84592E-16	8.35267E-15	2.02970E-09	2.73E-11
Am(OH)2+	(after_Cm(III))	2.53870E-15	1.03053E-15	0.4059	1.14231E-16	2.48090E-15	6.87245E-10	4.55E-10
AmOH++	(after_Cm(III))	2.16124E-16	4.50036E-18	2.0823E-02	9.72469E-18	2.11203E-16	5.49143E-11	2.41E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.56750E-01	9.69014E-01	1.013	2.63827E+00	5.38283E+01	9.69728E+05	
NaAm(CO3)2.6H2O(c)		8.18236E+01	1.00000E+00	1.000	3.88900E+00	7.93467E+01	3.92052E+07	
Na+	Na+	1.65251E+00	9.56629E-01	0.5789	7.85420E-02	1.60248E+00	3.68407E+04	
CO3=	CO3=	7.95637E-01	3.70954E-02	4.6624E-02	3.78158E-02	7.71552E-01	4.63002E+04	
HCO3-	HCO3-	6.04112E-02	2.40751E-02	0.3389	2.87129E-03	5.85825E-02	3.57453E+03	
OH-	OH-	6.77071E-04	3.86379E-04	0.5707	3.21805E-05	6.56575E-04	1.11666E+01	-1.24E-10
Am(CO3)3=-	Am(CO3)3=-	4.78225E-05	2.82614E-08	5.9138E-04	2.27295E-06	4.63748E-05	1.96178E+01	2.86E-11
CO2(aq)	CO2(aq)	8.34566E-07	1.16144E-06	1.392	3.96661E-08	8.09303E-07	3.56172E-02	-8.21E-10
Am(CO3)2-	Am(CO3)2-	3.11332E-09	1.00047E-09	0.3214	1.47973E-10	3.01907E-09	1.09598E-03	9.43E-12
H+	H+	6.02999E-11	2.52730E-11	0.4191	2.85599E-12	5.84745E-11	5.89364E-08	-2.93E-10
Am(OH)3(aq)	(1e-9m_minimum)	3.40984E-12	3.40984E-12	1.000	1.62066E-13	3.30662E-12	9.72219E-07	8.68E-10
AmCO3+	AmCO3+	1.37034E-12	5.09912E-13	0.3721	6.51307E-14	1.32885E-12	4.02655E-07	9.27E-12
Am+++	Am+++	1.73639E-14	7.73161E-19	2.1491E-05	8.25289E-16	1.68383E-14	4.09170E-09	5.03E-11
Am(OH)2+	(after_Cm(III))	2.98825E-15	1.11195E-15	0.3721	1.42028E-16	2.89779E-15	8.02730E-10	5.95E-10
AmOH++	(after_Cm(III))	2.81865E-16	3.96919E-18	1.4082E-02	1.33967E-17	2.73332E-16	7.10683E-11	3.23E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.43936E-01	9.60331E-01	1.017	2.84008E+00	5.33117E+01	9.60421E+05	
NaAm(CO3)2.6H2O(c)		7.60095E+01	1.00000E+00	1.000	3.88899E+00	7.30011E+01	3.60698E+07	
Na+	Na+	2.17890E+00	1.22126E+00	0.5605	1.11482E-02	2.09266E+00	4.81098E+04	
CO3=	CO3=	1.06076E+00	3.89196E-02	3.6690E-02	5.42731E-02	1.01877E+00	6.11357E+04	
HCO3-	HCO3-	5.62918E-02	1.73273E-02	0.3078	2.88015E-03	5.40639E-02	3.29882E+03	
OH-	OH-	8.01620E-04	4.74731E-04	0.5922	4.10145E-05	7.69892E-04	1.30938E+01	-1.39E-10
Am(CO3)3=-	Am(CO3)3=-	9.86519E-05	2.45322E-08	2.4867E-04	5.04748E-06	9.47473E-05	4.00807E+01	4.05E-11
CO2(aq)	CO2(aq)	5.17378E-07	7.99953E-07	1.346	2.64714E-08	4.96900E-07	2.18685E-02	-1.63E-09
Am(CO3)2-	Am(CO3)2-	2.86668E-09	8.27163E-10	0.2885	1.46672E-10	2.75322E-09	9.99469E-04	1.64E-11
H+	H+	5.09292E-11	2.03851E-11	0.4003	2.60577E-12	4.89135E-11	4.92999E-08	-6.65E-10
Am(OH)3(aq)	(1e-9m_minimum)	4.75043E-12	4.75043E-12	1.000	2.43053E-13	4.56241E-12	1.34145E-06	1.93E-09
AmCO3+	AmCO3+	1.17442E-12	4.01825E-13	0.3421	6.00885E-14	1.12793E-12	3.41775E-07	1.94E-11
Am+++	Am+++	3.67646E-14	2.80279E-19	7.6236E-06	1.88104E-15	3.53095E-14	8.58020E-09	8.95E-11
Am(OH)2+	(after_Cm(III))	3.68497E-15	1.26081E-15	0.3421	1.88540E-16	3.53912E-15	9.80389E-10	1.33E-09
AmOH++	(after_Cm(III))	3.81967E-16	3.66295E-18	9.5897E-03	1.95432E-17	3.66849E-16	9.53834E-11	7.14E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.28886E-01	9.49667E-01	1.022	3.12971E+00	5.26994E+01	9.49391E+05	
NaAm(CO3)2.6H2O(c)		6.89753E+01	1.00000E+00	1.000	3.88899E+00	6.54845E+01	3.23559E+07	
Na+	Na+	2.81575E+00	1.53675E+00	0.5458	1.58759E-01	2.67325E+00	6.14574E+04	

Figure 6.4.5 Edited Listing of the Output File FMT_AM_NA2CO3_QB0204.OUT
(Page 5 of 5)

CO3=-	CO3=	1.38144E+00	4.08310E-02	2.9557E-02	7.78889E-02	1.31153E+00	7.87038E+04	
HCO3-	HCO3-	5.12897E-02	1.44473E-02	0.2817	2.89183E-03	4.86940E-02	2.97116E+03	
OH-	OH-	9.34327E-04	5.90695E-04	0.6322	5.26795E-05	8.87041E-04	1.50862E+01	-2.03E-10
Am(CO3)3=-	Am(CO3)3=-	2.14490E-04	2.18707E-08	1.0197E-04	1.20934E-05	2.03635E-04	8.61430E+01	9.18E-11
CO2(aq)	CO2(aq)	3.05235E-07	5.36053E-07	1.756	1.72098E-08	2.89787E-07	1.27535E-02	-6.46E-09
Am(CO3)2-	Am(CO3)2-	2.69913E-09	7.02901E-10	0.2604	1.52183E-10	2.56253E-09	9.30246E-04	4.44E-11
H+	H+	4.17808E-11	1.62013E-11	0.3878	2.35570E-12	3.96663E-11	3.99797E-08	-2.93E-09
Am(OH)3(aq)	(1e-9m_minimum)	7.06537E-12	7.06537E-12	1.000	3.98362E-13	6.70780E-12	1.87224E-06	8.26E-09
AmCO3+	AmCO3+	1.02800E-12	3.25474E-13	0.3166	5.79607E-14	9.75969E-13	2.95728E-07	3.50E-11
Am+++	Am+++	7.72314E-14	2.16395E-19	2.8019E-06	4.35448E-15	7.33227E-14	1.78174E-08	1.99E-10
Am(OH)2+	(after_Cm(III))	4.76004E-15	1.50708E-15	0.3166	2.68382E-16	4.51913E-15	1.25187E-09	5.65E-09
AmOH++	(after_Cm(III))	5.27674E-16	3.51887E-18	6.6686E-03	2.97515E-17	5.00969E-16	1.30256E-10	2.97E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.12166E-01	9.36862E-01	1.027	3.54540E+00	5.20119E+01	9.37005E+05	
NaAm(CO3)2.6H2O(c)		6.08877E+01	1.00000E+00	1.000	3.88897E+00	5.70521E+01	2.81894E+07	
Na+	Na+	3.54797E+00	1.90244E+00	0.5362	2.26613E-01	3.32446E+00	7.64287E+04	
CO3=-	CO3=-	1.74997E+00	4.31374E-02	2.4650E-02	1.11772E-01	1.63973E+00	9.83987E+04	
HCO3-	HCO3-	4.55325E-02	1.18700E-02	0.2607	2.90821E-03	4.26642E-02	2.60324E+03	
OH-	OH-	1.08109E-03	7.49322E-04	0.6931	6.90507E-05	1.01299E-03	1.72282E+01	-1.16E-11
Am(CO3)3=-	Am(CO3)3=-	4.74303E-04	2.02485E-08	4.2691E-05	3.02943E-05	4.44242E-04	1.88004E+02	-6.42E-13
CO2(aq)	CO2(aq)	1.70762E-07	3.47188E-07	2.033	1.09068E-08	1.60005E-07	7.04179E-03	2.43E-11
Am(CO3)2-	Am(CO3)2-	2.59817E-09	6.15970E-10	0.2371	1.65948E-10	2.43450E-09	8.83767E-04	8.02E-14
H+	H+	3.30096E-11	1.23993E-11	0.3817	2.10836E-12	3.09302E-11	3.11745E-08	1.21E-11
Am(OH)3(aq)	(1e-9m_minimum)	1.13237E-11	1.13237E-11	1.000	7.23260E-13	1.06104E-11	3.11969E-06	-3.61E-11
AmCO3+	AmCO3+	9.13175E-13	2.69972E-13	0.2956	5.83255E-14	8.55649E-13	2.59269E-07	2.10E-13
Am+++	Am+++	1.53985E-13	1.69897E-19	1.1033E-06	9.83521E-15	1.44285E-13	3.50612E-08	-1.83E-11
Am(OH)2+	(after_Cm(III))	6.44051E-15	1.90408E-15	0.2956	4.11363E-16	6.03478E-15	1.67172E-09	-2.41E-11
AmOH++	(after_Cm(III))	7.31245E-16	3.50467E-18	4.7927E-03	4.67054E-17	6.85179E-16	1.78152E-10	-1.22E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.94701E-01	9.22025E-01	1.031	4.14209E+00	5.12847E+01	9.23904E+05	
NaAm(CO3)2.6H2O(c)		5.21159E+01	1.00000E+00	1.000	3.88892E+00	4.81501E+01	2.37909E+07	
Na+	Na+	4.34211E+00	3.12125E+00	0.5325	3.24011E-01	4.01169E+00	9.22279E+04	
CO3=-	CO3=-	2.14924E+00	4.60422E-02	2.1423E-02	1.60378E-01	1.98569E+00	1.19160E+05	
HCO3-	HCO3-	3.93018E-02	9.61279E-03	0.2446	2.93273E-03	3.63111E-02	2.21560E+03	
OH-	OH-	1.25373E-03	9.71938E-04	0.7752	9.35543E-05	1.15833E-03	1.97000E+01	-9.20E-12
Am(CO3)3=-	Am(CO3)3=-	1.02337E-03	1.95698E-08	1.9123E-05	7.63646E-05	9.45497E-04	3.99971E+02	-1.48E-11
CO2(aq)	CO2(aq)	9.09584E-08	2.16767E-07	2.383	6.78737E-09	8.40368E-08	3.69844E-03	3.79E-10
Am(CO3)2-	Am(CO3)2-	2.55510E-09	5.57765E-10	0.2183	1.90663E-10	2.36067E-09	8.56965E-04	-1.93E-11
H+	H+	2.50621E-11	9.55971E-12	0.3814	1.87015E-12	2.31550E-11	2.33379E-08	1.56E-10
Am(OH)3(aq)	(1e-9m_minimum)	1.96421E-11	1.96421E-11	1.000	1.46571E-12	1.81474E-11	5.33574E-06	-5.95E-10
AmCO3+	AmCO3+	8.20835E-13	2.29038E-13	0.2790	6.12512E-14	7.58372E-13	2.29794E-07	-8.62E-08
Am+++	Am+++	2.82283E-13	1.35044E-19	4.7840E-07	2.10642E-14	2.60803E-13	6.33750E-08	-1.24E-08
Am(OH)2+	(after_Cm(III))	9.12558E-15	2.54632E-15	0.2790	6.80956E-16	8.43115E-15	2.33555E-09	-4.34E-10
AmOH++	(after_Cm(III))	1.00631E-15	3.61331E-18	3.5907E-03	7.50912E-17	9.29730E-16	2.41737E-10	-2.84E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	8.77594E-01	9.05691E-01	1.032	4.99867E+00	5.05621E+01	9.10887E+05	
NaAm(CO3)2.6H2O(c)		4.31841E+01	1.00000E+00	1.000	3.88881E+00	3.93358E+01	1.94358E+07	
Na+	Na+	5.15071E+00	2.75210E+00	0.5343	4.63832E-01	4.69171E+00	1.07861E+05	
CO3=-	CO3=-	2.55501E+00	4.95808E-02	1.9405E-02	2.30084E-01	2.32733E+00	1.39661E+05	
HCO3-	HCO3-	3.29976E-02	7.68164E-03	0.2328	2.97150E-03	3.00571E-02	1.83400E+03	
Am(CO3)3=-	Am(CO3)3=-	2.07247E-03	1.97093E-08	9.5100E-06	1.86630E-04	1.88779E-03	7.98586E+02	-4.44E-13
OH-	OH-	1.46940E-03	1.28656E-03	0.8756	1.32322E-04	1.33845E-03	2.27635E+01	-1.13E-11
CO2(aq)	CO2(aq)	4.67113E-08	1.30860E-07	2.801	4.20645E-09	4.25487E-08	1.87256E-03	2.20E-11
Am(CO3)2-	Am(CO3)2-	2.56220E-09	5.21650E-10	0.2036	2.30731E-10	2.33387E-09	8.47239E-04	-2.78E-13
Am(OH)3(aq)	(1e-9m_minimum)	3.67428E-11	3.67428E-11	1.000	3.30876E-12	3.34686E-11	9.84049E-06	-3.33E-11
H+	H+	1.83838E-11	7.09400E-12	0.3859	1.65550E-12	1.67456E-11	1.68779E-08	1.06E-11
AmCO3+	AmCO3+	7.46933E-13	1.98920E-13	0.2663	6.72628E-14	6.80372E-13	2.06159E-07	-6.05E-13
Am+++	Am+++	4.68303E-13	1.08915E-19	2.3257E-07	4.21716E-14	4.26571E-13	1.03657E-07	-1.93E-12
Am(OH)2+	(after_Cm(III))	1.35117E-14	3.59838E-15	0.2663	1.21676E-15	1.23076E-14	3.40939E-09	-2.26E-11
AmOH++	(after_Cm(III))	1.36966E-15	3.85752E-18	2.8164E-03	1.23340E-16	1.24760E-15	3.24385E-10	-2.77E-09

Total G/RT= -6.00840876E+03

TITRATE file name is WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AM_NA2CO3_QB0204.TITRATE;1

Figure 6.4.6 Edited Listing of the Output File FMT_AM_NA2CO3_QB0204.TITRATE
(Page 1 of 3)

Benchmark: Solubility of NaAm(CO3)2.6H2O(s) versus Na2CO3
FMT_pH_970407.chemdat
Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5=== by analogy

FMT V2.4

Titrant Volumes per Grid Block, in milliliters

1	0.000000 mL
2	0.030000 mL
3	0.043053 mL
4	0.061786 mL
5	0.088669 mL
6	0.127250 mL
7	0.182617 mL
8	0.262074 mL
9	0.376104 mL
10	0.539749 mL
11	0.774597 mL
12	1.111628 mL
13	1.595303 mL
14	2.289428 mL
15	3.285571 mL
16	4.715141 mL
17	6.766725 mL
18	9.710964 mL
19	13.936258 mL
20	20.000000 mL

Titration Results, molal

0)	H2O	Na+	H+
1)	2.17475E+00	7.35404E-02	9.78995E-09
2)	2.17874E+00	8.99454E-02	1.09416E-09
3)	2.18058E+00	9.75254E-02	7.97618E-10
4)	2.18323E+00	1.08381E-01	5.87153E-10
5)	2.18702E+00	1.23914E-01	4.38177E-10
6)	2.19246E+00	1.46112E-01	3.32468E-10
7)	2.20028E+00	1.77776E-01	2.56984E-10
8)	2.21149E+00	2.22827E-01	2.02570E-10
9)	2.22759E+00	2.86686E-01	1.62885E-10
10)	2.25069E+00	3.76735E-01	1.33550E-10
11)	2.28384E+00	5.02782E-01	1.11528E-10
12)	2.33141E+00	6.77411E-01	9.46502E-11
13)	2.39968E+00	9.15924E-01	8.12967E-11
14)	2.49766E+00	1.23544E+00	7.01860E-11
15)	2.63827E+00	1.65251E+00	6.02999E-11
16)	2.84008E+00	2.17890E+00	5.09292E-11
17)	3.12971E+00	2.81575E+00	4.17808E-11
18)	3.54540E+00	3.54797E+00	3.30096E-11
19)	4.14209E+00	4.34211E+00	2.50621E-11
20)	4.99867E+00	5.15071E+00	1.83838E-11

0)	OH-	HCO3-	CO3=	CO2 (aq)
1)	1.66896E-06	7.17417E-02	8.98457E-04	9.00252E-04
2)	1.58994E-05	7.21629E-02	8.88279E-03	9.40193E-05
3)	2.23778E-05	7.21634E-02	1.26691E-02	6.64681E-05
4)	3.14417E-05	7.21240E-02	1.81119E-02	4.69474E-05
5)	4.39885E-05	7.20389E-02	2.59144E-02	3.31839E-05
6)	6.11657E-05	7.18965E-02	3.70755E-02	2.34863E-05
7)	8.44063E-05	7.16781E-02	5.30045E-02	1.66399E-05
8)	1.15444E-04	7.13556E-02	7.56746E-02	1.17889E-05
9)	1.56269E-04	7.08885E-02	1.07816E-01	8.33757E-06
10)	2.08970E-04	7.02200E-02	1.53147E-01	5.87291E-06
11)	2.75373E-04	6.92736E-02	2.16608E-01	4.10845E-06
12)	3.56497E-04	6.79492E-02	3.04539E-01	2.84400E-06
13)	4.51965E-04	6.61233E-02	4.24653E-01	1.93841E-06
14)	5.59798E-04	6.36561E-02	5.85572E-01	1.29194E-06
15)	6.77071E-04	6.04112E-02	7.95637E-01	8.34566E-07

Figure 6.4.6 Edited Listing of the Output File FMT_AM_NA2CO3_QB0204.TITRATE
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16)	8.01620E-04	5.62918E-02	1.06076E+00	5.17378E-07		
17)	9.34327E-04	5.12897E-02	1.38144E+00	3.05235E-07		
18)	1.08109E-03	4.55325E-02	1.74997E+00	1.70762E-07		
19)	1.25373E-03	3.93018E-02	2.14924E+00	9.09584E-08		
20)	1.46940E-03	3.29976E-02	2.55501E+00	4.67113E-08		
0)	Am+++					
1)	1.07521E-12					
2)	1.56248E-14					
3)	8.91945E-15					
4)	5.33803E-15					
5)	3.40276E-15					
6)	2.34605E-15					
7)	1.77550E-15					
8)	1.49587E-15					
9)	1.42149E-15					
10)	1.54132E-15					
11)	1.92359E-15					
12)	2.77209E-15					
13)	4.58589E-15					
14)	8.54730E-15					
15)	1.73639E-14					
16)	3.67646E-14					
17)	7.72314E-14					
18)	1.53985E-13					
19)	2.82283E-13					
20)	4.68303E-13					
0)	AmCO3+	Am(CO3)2-	Am(CO3)3=-	AmOH++	Am(OH)2+	Am(OH)3(aq)
1)	1.03314E-09	1.83893E-08	3.73302E-08	7.24537E-15	2.94848E-15	2.39019E-14
2)	9.96774E-11	1.59643E-08	3.38344E-07	8.02173E-16	2.71400E-15	1.96554E-13
3)	6.86904E-11	1.50896E-08	4.67003E-07	5.86883E-16	2.64109E-15	2.62199E-13
4)	4.70352E-11	1.40257E-08	6.40835E-07	4.35432E-16	2.55428E-15	3.44128E-13
5)	3.20605E-11	1.27915E-08	8.72970E-07	3.29661E-16	2.45475E-15	4.42517E-13
6)	2.18002E-11	1.14348E-08	1.18108E-06	2.56332E-16	2.34681E-15	5.56419E-13
7)	1.48331E-11	1.00270E-08	1.59116E-06	2.06150E-16	2.23808E-15	6.84492E-13
8)	1.01437E-11	8.64846E-09	2.14541E-06	1.72813E-16	2.13893E-15	8.26433E-13
9)	7.01207E-12	7.37109E-09	2.91833E-06	1.52262E-16	2.06146E-15	9.84741E-13
10)	4.93366E-12	6.24537E-09	4.05012E-06	1.42203E-16	2.01877E-15	1.16648E-12
11)	3.55937E-12	5.29600E-09	5.81837E-06	1.41872E-16	2.02515E-15	1.38518E-12
12)	2.65131E-12	4.52512E-09	8.79928E-06	1.52035E-16	2.09750E-15	1.66391E-12
13)	2.04930E-12	3.91931E-09	1.42468E-05	1.75227E-16	2.25805E-15	2.04113E-12
14)	1.64616E-12	3.45677E-09	2.50150E-05	2.16124E-16	2.53870E-15	2.58312E-12
15)	1.37034E-12	3.11332E-09	4.78225E-05	2.81865E-16	2.98825E-15	3.40984E-12
16)	1.17442E-12	2.86668E-09	9.86519E-05	3.81967E-16	3.68497E-15	4.75043E-12
17)	1.02800E-12	2.69913E-09	2.14490E-04	5.27674E-16	4.76004E-15	7.06537E-12
18)	9.13175E-13	2.59817E-09	4.74303E-04	7.31245E-16	6.44051E-15	1.13237E-11
19)	8.20835E-13	2.55510E-09	1.02337E-03	1.00631E-15	9.12558E-15	1.96421E-11
20)	7.46933E-13	2.56220E-09	2.07247E-03	1.36966E-15	1.35117E-14	3.67428E-11
0)	IonicStrength	Titrvol,ml	pH		pmH	
1)	7.44390E-02	0.000000000E+00	8.122		8.009	
2)	9.88292E-02	3.000000000E-02	9.087		8.961	
3)	1.10196E-01	4.305316402E-02	9.230		9.098	
4)	1.26495E-01	6.178583106E-02	9.371		9.231	
5)	1.49831E-01	8.866918395E-02	9.508		9.358	
6)	1.83191E-01	0.127249631	9.641		9.478	
7)	2.30786E-01	0.182616641	9.768		9.590	
8)	2.98508E-01	0.262074139	9.889		9.693	
9)	3.94511E-01	0.376104030	10.01		9.788	
10)	5.29894E-01	0.539748950	10.12		9.874	
11)	7.19408E-01	0.774596669	10.22		9.953	
12)	9.81977E-01	1.11162791	10.32		10.02	
13)	1.34062E+00	1.59530330	10.42		10.09	
14)	1.82108E+00	2.28942849	10.51		10.15	
15)	2.44829E+00	3.28557134	10.60		10.22	
16)	3.23995E+00	4.71514139	10.69		10.29	
17)	4.19784E+00	6.76672518	10.79		10.38	

Figure 6.4.6 Edited Listing of the Output File FMT_AM_NA2CO3_QB0204.TITRATE
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18)	5.29936E+00	9.71096431	10.90	10.48
19)	6.49442E+00	13.9362580	11.02	10.60
20)	7.71194E+00	20.0000000	11.15	10.74

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHCO3_QB0204.OUT
(Page 1 of 10)

INPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AM_NAHCO3.IN;1
 INGUESS file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AM_NAHCO3.INGUESS;1
 OUTPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AM_NAHCO3_QB0204.OUT;1
 CHEMDAT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
 Temperature is Hard Coded as 298.15K
 Benchmark: Solubility of NaAm(CO3)2.6H2O(s) versus NaHCO3 FMT V2.4
 FMT_ph_970407.chemdat.
 Added Th(CO3)5-Cl(-Na) Pzrms, assigned K+-Th(CO3)5== by analogy

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.57855E-01	9.63166E-01	1.006	5.55087E+01	5.35890E+01	9.65416E+05	
NaHCO3	1.00000E+01	1.00000E+00	1.000	1.00000E+01	9.65416E+00	8.11016E+05	
Na+	1.22119E+00	6.45370E-01	0.5285	1.22119E+00	1.17895E+00	2.71039E+04	
CO2(aq)	1.82328E-02	2.32768E-02	1.277	1.82328E-02	1.76022E-02	7.74670E+02	
HCO3-	1.18472E+00	6.12584E-01	0.5171	1.18472E+00	1.14375E+00	6.97883E+04	1.20E-08
CO3=	1.82320E-02	1.66686E-03	9.1425E-02	1.82320E-02	1.76014E-02	1.05625E+03	-4.18E-08
OH-	6.34107E-07	5.76799E-07	0.6915	6.34107E-07	8.05261E-07	1.36953E-02	7.89E-08
H+	3.25446E-08	1.68274E-08	0.5171	3.25446E-08	3.14191E-08	3.16673E-05	-7.95E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.97357E-01	9.97557E-01	1.000	5.58797E+01	5.54390E+01	9.98744E+05	
NaAm(CO3)2.6H2O(c)	9.92624E+01	1.00000E+00	1.000	9.92606E+01	9.91378E+01	4.89839E+07	
Na+	7.35404E-02	5.70177E-02	0.7753	7.40320E-02	7.34481E-02	1.68855E+03	
HCO3-	7.17417E-02	5.54720E-02	0.7732	7.22213E-02	7.16516E-02	4.37197E+03	
CO2(aq)	9.00252E-04	9.13591E-04	1.015	9.06270E-04	8.99121E-04	3.95702E+01	
CO3=	8.98457E-04	3.36242E-04	0.3742	9.04463E-04	8.97329E-04	5.38480E+01	-5.79E-08
OH-	1.66896E-06	1.33078E-06	0.7974	1.68012E-06	1.66687E-06	2.83489E-02	1.35E-07
Am(CO3)3=-	3.73302E-08	3.61342E-09	9.6796E-02	3.75797E-08	3.72833E-08	1.57719E-02	1.17E-07
Am(CO3)2=-	1.83893E-08	1.41023E-08	0.7669	1.85122E-08	1.83662E-08	6.66727E-03	1.94E-08
H+	9.78996E-09	7.55393E-09	0.7716	9.85540E-09	9.77766E-09	9.85491E-06	-1.39E-07
AmCO3+	1.03314E-09	7.92958E-10	0.7675	1.04004E-09	1.03184E-09	3.12656E-04	-9.70E-08
Am+++	1.07521E-12	6.40206E-14	5.9542E-02	1.08240E-12	1.07386E-12	2.60949E-07	-2.44E-07
Am(OH)3(aq)	2.39019E-14	2.39019E-14	1.000	2.40617E-14	2.38719E-14	7.01886E-09	1.98E-07
AmOH++	7.24537E-15	2.34540E-15	0.3237	7.29380E-15	7.23627E-15	1.88148E-09	-8.75E-08
Am(OH)2+	2.94848E-15	2.26304E-15	0.7675	2.96819E-15	2.94478E-15	8.15747E-10	5.85E-08
AmOHC03(c)	1.07268E-03	1.00000E+00	1.000	1.07985E-03	1.07134E-03	3.42845E+02	-9.39E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.97357E-01	9.97557E-01	1.000	2.17475E+00	5.54390E+01	9.98744E+05	
NaAm(CO3)2.6H2O(c)	9.92624E+01	1.00000E+00	1.000	3.88896E+00	9.91378E+01	4.89839E+07	
Na+	7.35404E-02	5.70177E-02	0.7753	2.88121E-03	7.34481E-02	1.68855E+03	
HCO3-	7.17417E-02	5.54720E-02	0.7732	2.81074E-03	7.16516E-02	4.37197E+03	
CO2(aq)	9.00252E-04	9.13591E-04	1.015	3.52705E-05	8.99121E-04	3.95702E+01	
AmOHC03(c)	1.07268E-03	1.00000E+00	1.000	4.20261E-05	1.07134E-03	3.42845E+02	-1.11E-08
CO3=	8.98457E-04	3.36242E-04	0.3742	3.52002E-05	8.97329E-04	5.38480E+01	-6.99E-08
OH-	1.66896E-06	1.33078E-06	0.7974	6.53875E-08	1.66687E-06	2.83489E-02	1.58E-07
Am(CO3)3=-	3.73302E-08	3.61342E-09	9.6796E-02	1.46254E-09	3.72833E-08	1.57719E-02	1.37E-07
Am(CO3)2=-	1.83893E-08	1.41023E-08	0.7669	7.20466E-10	1.83662E-08	6.66727E-03	2.31E-08
H+	9.78996E-09	7.55393E-09	0.7716	3.83556E-10	9.77766E-09	9.85491E-06	-1.63E-07
AmCO3+	1.03314E-09	7.92958E-10	0.7675	4.04767E-11	1.03184E-09	3.12656E-04	-1.13E-07
Am+++	1.07521E-12	6.40206E-14	5.9542E-02	4.21253E-14	1.07386E-12	2.60949E-07	-2.85E-07
Am(OH)3(aq)	2.39019E-14	2.39019E-14	1.000	9.36442E-16	2.38719E-14	7.01886E-09	2.33E-07
AmOH++	7.24537E-15	2.34540E-15	0.3237	2.83863E-16	7.23627E-15	1.88148E-09	-1.02E-07
Am(OH)2+	2.94848E-15	2.26304E-15	0.7675	1.15517E-16	2.94478E-15	8.15747E-10	6.98E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.96209E-01	9.96531E-01	1.000	2.18104E+00	5.53855E+01	9.97781E+05	
NaAm(CO3)2.6H2O(c)	9.89773E+01	1.00000E+00	1.000	3.88900E+00	9.87577E+01	4.87961E+07	
Na+	1.05620E-01	7.87685E-02	0.7458	4.14999E-03	1.05385E-01	2.42278E+03	
HCO3-	1.02969E-01	7.65109E-02	0.7430	4.04585E-03	1.02741E-01	6.26895E+03	
CO2(aq)	1.32599E-03	1.35403E-03	1.021	5.21006E-05	1.32305E-03	5.82271E+01	
CO3=	1.32426E-03	4.31952E-04	0.3262	5.20325E-05	1.32132E-03	7.92913E+01	-1.05E-09
OH-	1.59766E-06	1.23820E-06	0.7750	6.27751E-08	1.59412E-06	2.71116E-02	-3.42E-10
Am(CO3)3=-	4.80079E-08	3.38096E-09	7.0425E-02	1.88632E-09	4.79014E-08	2.02636E-02	-7.24E-10
Am(CO3)2=-	1.39822E-08	1.02713E-08	0.7346	5.49385E-10	1.39511E-08	5.06452E-03	4.97E-12
H+	1.09451E-08	8.10359E-09	0.7410	4.30053E-10	1.09208E-08	1.10071E-05	7.27E-10
AmCO3+	6.11347E-10	4.49578E-10	0.7354	2.40210E-11	6.09991E-10	1.84833E-04	7.39E-10
Am+++	7.66585E-13	2.82548E-14	3.6858E-02	3.01205E-14	7.64884E-13	1.85867E-07	9.62E-10
Am(OH)3(aq)	8.49698E-15	8.49698E-15	1.000	3.33862E-16	8.47813E-15	2.49276E-09	-7.17E-10
AmOH++	3.58638E-15	9.63109E-16	0.2685	1.40915E-16	3.57842E-15	9.30415E-10	-2.66E-08
Am(OH)2+	1.17576E-15	8.64643E-16	0.7354	4.61979E-17	1.17315E-15	3.24981E-10	1.34E-11

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.95032E-01	9.95490E-01	1.000	2.18754E+00	5.53307E+01	9.96794E+05	
NaAm(CO3)2.6H2O(c)	9.86832E+01	1.00000E+00	1.000	3.88900E+00	9.83668E+01	4.86030E+07	
Na+	1.38567E-01	1.00108E-01	0.7224	5.46079E-03	1.38123E-01	3.17542E+03	
HCO3-	1.35023E-01	9.71026E-02	0.7192	5.32110E-03	1.34590E-01	8.21228E+03	

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHC03_QB0204.OUT
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CO2 (aq)	CO2 (aq)	1.77318E-03	1.82301E-03	1.028	6.98791E-05	1.76749E-03	7.77871E+01		
CO3=	CO3=	1.77150E-03	5.17403E-04	0.2921	6.98127E-05	1.76582E-03	1.05965E+02	-4.80E-10	
OH-	OH-	1.53942E-06	1.16741E-06	0.7583	6.06670E-08	1.53449E-06	2.60975E-02	-7.11E-10	
Am(CO3)3--	Am(CO3)3--	5.87747E-08	3.20658E-09	5.4557E-02	2.31625E-09	5.85863E-08	2.47836E-02	-7.24E-10	
H+	H+	1.19886E-08	8.59316E-09	0.7168	4.72458E-10	1.19502E-08	1.20446E-05	7.11E-10	
Am(CO3)2-	Am(CO3)2-	1.14745E-08	8.13269E-09	0.7088	4.52198E-10	1.14377E-08	4.15210E-03	4.62E-12	
AmCO3+	AmCO3+	4.18762E-10	2.97179E-10	0.7097	1.65029E-11	4.17419E-10	1.26482E-04	7.28E-10	
Am+++	Am+++	6.33388E-13	1.55923E-14	2.4617E-02	2.49611E-14	6.31357E-13	1.53420E-07	1.45E-09	
Am(OH)3 (aq)	(1e-9m_minimum)	3.92992E-15	3.92992E-15	1.000	1.54874E-16	3.91732E-15	1.15178E-09	-6.82E-10	
AmOH++	(after_Cm(III))	2.18166E-15	5.01104E-16	0.2297	8.59770E-17	2.17467E-15	5.65430E-10	7.38E-10	
Am(OH)2+	(after_Cm(III))	5.97683E-16	4.24153E-16	0.7097	2.35540E-17	5.95766E-16	1.65036E-10	2.88E-11	

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor	
H2O	WATER	9.93865E-01	9.94466E-01	1.001	2.19404E+00	5.52763E+01	9.95814E+05	
NaAm(CO3)2.6H2O(c)		9.83908E+01	1.00000E+00	1.000	3.88900E+00	9.79790E+01	4.84114E+07	
Na+	Na+	1.71320E-01	1.20549E-01	0.7036	6.77160E-03	1.70603E-01	3.92212E+03	
HCO3-	HCO3-	1.66871E-01	1.16786E-01	0.6999	6.59576E-03	1.66173E-01	1.013394E+04	
CO2 (aq)	CO2 (aq)	2.22511E-03	2.30267E-03	1.035	8.79498E-05	2.21580E-03	9.75168E+01	
CO3=	CO3=	2.22346E-03	5.93133E-04	0.2668	8.78847E-05	2.21416E-03	1.32870E+02	-1.93E-10
OH-	OH-	1.49079E-06	1.11518E-06	0.7456	5.89249E-08	1.48455E-06	2.52481E-02	-6.60E-09
Am(CO3)3--	Am(CO3)3--	6.94575E-08	3.07152E-09	4.4222E-02	2.74538E-09	6.91668E-08	2.92595E-02	-6.63E-09
H+	H+	1.29307E-08	9.01549E-09	0.6972	5.11098E-10	1.28766E-08	1.29783E-05	6.45E-09
Am(CO3)2-	Am(CO3)2-	9.88188E-09	6.79552E-09	0.6877	3.90592E-10	9.84052E-09	3.57229E-03	1.36E-11
AmCO3+	AmCO3+	3.14538E-10	2.16613E-10	0.6887	1.24324E-11	3.13221E-10	9.49089E-05	6.63E-09
Am+++	Am+++	5.67790E-13	9.91411E-15	1.7461E-02	2.24425E-14	5.65413E-13	1.37395E-07	1.33E-08
Am(OH)3 (aq)	(1e-9m_minimum)	2.15712E-15	2.15712E-15	1.000	8.52623E-17	2.14809E-15	6.31585E-10	-6.07E-09
AmOH++	(after_Cm(III))	1.50771E-15	3.03380E-16	0.2012	5.95939E-17	1.50140E-15	3.90375E-10	6.48E-09
Am(OH)2+	(after_Cm(III))	3.55047E-16	2.44510E-16	0.6887	1.40336E-17	3.53561E-16	9.79416E-11	3.76E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor	
H2O	WATER	9.92708E-01	9.93455E-01	1.001	2.20054E+00	5.52224E+01	9.94843E+05	
NaAm(CO3)2.6H2O(c)		9.81002E+01	1.00000E+00	1.000	3.88900E+00	9.75942E+01	4.82212E+07	
Na+	Na+	2.03879E-01	1.40254E-01	0.6879	8.08241E-03	2.02828E-01	4.66296E+03	
HCO3-	HCO3-	1.98520E-01	1.35725E-01	0.6837	7.86997E-03	1.97497E-01	1.20507E+04	
CO2 (aq)	CO2 (aq)	2.68013E-03	2.79167E-03	1.042	1.06249E-04	2.66631E-03	1.17344E+02	
CO3=	CO3=	2.67852E-03	6.1458E-04	0.2469	1.06185E-04	2.66470E-03	1.59907E+02	8.65E-09
OH-	OH-	1.44865E-06	1.06556E-06	0.7356	5.74289E-08	1.44118E-06	2.45105E-02	-2.32E-07
Am(CO3)3--	Am(CO3)3--	8.01727E-08	2.96210E-09	3.6947E-02	3.17830E-09	7.97592E-08	3.37403E-02	-3.41E-07
H+	H+	1.37994E-08	9.39528E-09	0.6808	5.47050E-10	1.37282E-08	1.38367E-05	2.32E-07
Am(CO3)2-	Am(CO3)2-	8.77289E-09	5.67651E-09	0.6698	3.47785E-10	8.72765E-09	3.16830E-03	3.89E-10
AmCO3+	AmCO3+	2.50354E-10	1.67969E-10	0.6709	9.92483E-12	2.49063E-10	7.54684E-05	2.39E-07
Am+++	Am+++	5.33478E-13	6.89364E-15	1.2922E-02	2.11487E-14	5.30726E-13	1.28966E-07	-2.18E-07
Am(OH)3 (aq)	(1e-9m_minimum)	1.32125E-15	1.32125E-15	1.000	5.23784E-17	1.31443E-15	3.86472E-10	-2.18E-07
AmOH++	(after_Cm(III))	1.12796E-15	2.02218E-16	0.1793	4.47157E-17	1.12214E-15	2.91764E-10	2.46E-07
Am(OH)2+	(after_Cm(III))	2.32859E-16	1.56232E-16	0.6709	9.23127E-18	2.31658E-16	6.41727E-11	1.38E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor	
H2O	WATER	9.91560E-01	9.92456E-01	1.001	2.20704E+00	5.51689E+01	9.93879E+05	
NaAm(CO3)2.6H2O(c)		9.78112E+01	1.00000E+00	1.000	3.88900E+00	9.72125E+01	4.80326E+07	
Na+	Na+	2.36246E-01	1.59338E-01	0.6745	9.39321E-03	2.34800E-01	5.39800E+03	
HCO3-	HCO3-	2.29974E-01	1.54035E-01	0.6698	9.14380E-03	2.28566E-01	1.39464E+04	
CO2 (aq)	CO2 (aq)	3.13717E-03	3.28896E-03	1.048	1.24735E-04	3.11797E-03	1.37221E+02	
CO3=	CO3=	3.13559E-03	7.23876E-04	0.2309	1.24672E-04	3.11640E-03	1.87012E+02	7.01E-09
OH-	OH-	1.41121E-06	1.02646E-06	0.7274	5.61102E-08	1.40257E-06	2.38540E-02	-2.08E-07
Am(CO3)3--	Am(CO3)3--	9.10035E-08	2.87065E-09	3.1544E-02	3.61832E-09	9.04464E-08	3.82613E-02	-2.89E-07
H+	H+	1.46119E-08	9.74334E-09	0.6668	5.80971E-10	1.45224E-08	1.46371E-05	2.09E-07
Am(CO3)2-	Am(CO3)2-	7.95220E-09	5.20401E-09	0.6544	3.16181E-10	7.90352E-09	2.86912E-03	3.34E-10
AmCO3+	AmCO3+	2.07335E-10	1.35921E-10	0.6556	8.24369E-12	2.06066E-10	6.24398E-05	2.14E-07
Am+++	Am+++	5.16283E-13	5.09736E-15	9.8732E-03	2.05276E-14	5.13123E-13	1.24689E-07	-1.48E-07
AmOH++	(after_Cm(III))	8.90423E-16	1.44040E-16	0.1618	3.54034E-17	8.84972E-16	2.30099E-10	2.22E-07
Am(OH)3 (aq)	(1e-9m_minimum)	8.73325E-16	8.73325E-16	1.000	3.47236E-17	8.67979E-16	2.55205E-10	-1.96E-07
Am(OH)2+	(after_Cm(III))	1.63523E-16	1.07200E-16	0.6556	6.50173E-18	1.62522E-16	4.50211E-11	1.26E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor	
H2O	WATER	9.90421E-01	9.91469E-01	1.001	2.21354E+00	5.51158E+01	9.92922E+05	
NaAm(CO3)2.6H2O(c)		9.75240E+01	1.00000E+00	1.000	3.88900E+00	9.68337E+01	4.78455E+07	
Na+	Na+	2.68424E-01	1.77881E-01	0.6627	1.07040E-02	2.66524E-01	6.12732E+03	
HCO3-	HCO3-	2.61234E-01	1.71800E-01	0.6576	1.04173E-02	2.59385E-01	1.58269E+04	
CO2 (aq)	CO2 (aq)	3.59552E-03	3.79382E-03	1.055	1.43380E-04	3.57007E-03	1.57118E+02	
CO3=	CO3=	3.59396E-03	7.81419E-04	0.2174	1.43318E-04	3.56852E-03	2.14144E+02	5.89E-09
OH-	OH-	1.37736E-06	9.92496E-07	0.7206	5.49254E-08	1.36761E-06	2.32593E-02	-1.90E-07
Am(CO3)3--	Am(CO3)3--	1.02014E-07	2.79243E-09	2.7373E-02	4.06806E-09	1.01292E-07	4.28494E-02	-2.54E-07
H+	H+	1.53796E-08	1.00668E-08	0.6546	6.13298E-10	1.52708E-08	1.53914E-05	1.91E-07
Am(CO3)2-	Am(CO3)2-	7.31802E-09	4.68942E-09	0.6408	2.91823E-10	7.26622E-09	2.63777E-03	2.93E-10
AmCO3+	AmCO3+	1.76725E-10	1.13462E-10	0.6420	7.04731E-12	1.75474E-10	5.31702E-05	1.97E-07
Am+++	Am+++	5.09607E-13	3.94172E-15	7.7348E-03	2.03218E-14	5.06000E-13	1.22958E-07	1.36E-07
AmOH++	(after_Cm(III))	7.30571E-16	1.07698E-16	0.1474	2.91333E-17	7.25400E-16	1.88609E-10	2.04E-07
Am(OH)3 (aq)	(1e-9m_minimum)	6.10481E-16	6.10481E-16	1.000	2.43444E-17	6.06160E-16	1.78224E-10	-1.79E-07
Am(OH)2+	(after_Cm(III))	1.20713E-16	7.75008E-17	0.6420	4.81372E-18	1.19859E-16	3.32026E-11	1.18E-08

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHC03_QB0204.OUT
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Table with 8 columns: Species Name, Molality, Activity, Act Coef, Total Moles, Molarity, mg/liter, Descriptor. Rows include H2O, NaAm(CO3)2.6H2O(c), Na+, HCO3-, CO2(aq), CO3=, OH-, Am(CO3)3=, H+, Am(CO3)2-, AmCO3+, AmOH++, Am(OH)3(aq), Am(OH)2+.

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Table with 8 columns: Species Name, Molality, Activity, Act Coef, Total Moles, Molarity, mg/liter, Descriptor. Rows include H2O, NaAm(CO3)2.6H2O(c), Na+, HCO3-, CO2(aq), CO3=, OH-, Am(CO3)3=, H+, Am(CO3)2-, AmCO3+, AmOH++, Am(OH)3(aq), Am(OH)2+.

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Table with 8 columns: Species Name, Molality, Activity, Act Coef, Total Moles, Molarity, mg/liter, Descriptor. Rows include H2O, NaAm(CO3)2.6H2O(c), Na+, HCO3-, CO2(aq), CO3=, OH-, Am(CO3)3=, H+, Am(CO3)2-, AmCO3+, AmOH++, Am(OH)3(aq), Am(OH)2+.

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Table with 8 columns: Species Name, Molality, Activity, Act Coef, Total Moles, Molarity, mg/liter, Descriptor. Rows include H2O, NaAm(CO3)2.6H2O(c), Na+, HCO3-, CO2(aq), CO3=, OH-, Am(CO3)3=, H+, Am(CO3)2-, AmCO3+, AmOH++, Am(OH)3(aq), Am(OH)2+.

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Table with 8 columns: Species Name, Molality, Activity, Act Coef, Total Moles, Molarity, mg/liter, Descriptor. Rows include H2O, NaAm(CO3)2.6H2O(c), Na+, HCO3-, CO2(aq), CO3=, OH-, Am(CO3)3=, H+, Am(CO3)2-.

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHCO3_QB0204.OUT
(Page 4 of 10)

AmCO3+		1.02094E-10	6.03885E-11	0.5915	4.13102E-12	1.00894E-10	3.05719E-05	1.84E-07
Am+++	Am+++	5.52149E-13	1.61182E-15	2.9192E-03	2.23416E-14	5.45661E-13	1.32596E-07	3.65E-07
AmOH++	(after_Cm(III))	3.77502E-16	3.89369E-17	0.1021	1.52748E-17	3.73066E-16	9.69999E-11	1.91E-07
Am(OH)3(aq)	(1e-9m_minimum)	1.67269E-16	1.67269E-16	1.000	6.76818E-18	1.65303E-16	4.86027E-11	-1.67E-07
Am(OH)2+	(after_Cm(III))	4.10258E-17	2.42668E-17	0.5915	1.66003E-18	4.05438E-17	1.12312E-11	1.16E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.83780E-01	9.85742E-01	1.002	2.25255E+00	5.48057E+01	9.87336E+05	
NaAm(CO3)2.6H2O(c)		9.58351E+01	1.00000E+00	1.000	3.88900E+00	9.46215E+01	4.67524E+07	
Na+	Na+	4.57586E-01	2.80642E-01	0.6133	1.85689E-02	4.51791E-01	1.03866E+04	
HCO3-	HCO3-	4.44883E-01	2.69793E-01	0.6064	1.80534E-02	4.39249E-01	2.68017E+04	
CO2(aq)	CO2(aq)	6.35184E-03	6.96057E-03	1.096	2.57758E-04	6.27140E-03	7.6003E+02	
CO3=	CO3=	6.35037E-03	1.05644E-03	0.1664	2.57698E-04	6.26995E-03	3.76254E+02	5.20E-09
OH-	OH-	1.21921E-06	8.49509E-07	0.6968	4.94719E-08	1.20368E-06	2.04713E-02	-1.81E-07
Am(CO3)3=	Am(CO3)3=	1.74377E-07	2.47752E-09	1.4208E-02	7.07624E-09	1.72169E-07	7.28322E-02	-2.40E-07
H+	H+	1.93845E-08	1.16933E-08	0.6032	7.86623E-10	1.91390E-08	1.92902E-05	1.82E-07
Am(CO3)2-	Am(CO3)2-	5.28635E-09	3.07747E-09	0.5822	2.14521E-10	5.21941E-09	1.89474E-03	2.18E-10
AmCO3+	AmCO3+	9.43600E-11	5.50758E-11	0.5837	3.82914E-12	9.31650E-11	2.82298E-05	1.87E-07
Am+++	Am+++	5.69362E-13	1.41526E-15	2.4857E-03	2.31048E-14	5.62151E-13	1.36603E-07	3.75E-07
AmOH++	(after_Cm(III))	3.44302E-16	3.30976E-17	9.6130E-02	1.39718E-17	3.39942E-16	8.83873E-11	1.95E-07
Am(OH)3(aq)	(1e-9m_minimum)	1.37448E-16	1.37448E-16	1.000	5.57766E-18	1.35707E-16	3.99010E-11	-1.70E-07
Am(OH)2+	(after_Cm(III))	3.49270E-17	2.03861E-17	0.5837	1.41734E-18	3.44847E-17	9.55276E-12	1.19E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.82704E-01	9.84815E-01	1.002	2.25905E+00	5.47554E+01	9.86430E+05	
NaAm(CO3)2.6H2O(c)		9.55593E+01	1.00000E+00	1.000	3.88900E+00	9.42626E+01	4.65751E+07	
Na+	Na+	4.88478E-01	2.96657E-01	0.6073	1.98797E-02	4.81849E-01	1.10776E+04	
HCO3-	HCO3-	4.74858E-01	2.85001E-01	0.6002	1.93254E-02	4.68414E-01	2.85813E+04	
CO2(aq)	CO2(aq)	6.81036E-03	7.50929E-03	1.103	2.77163E-04	6.71794E-03	2.95655E+02	
CO3=	CO3=	6.80890E-03	1.09379E-03	0.1606	2.77103E-04	6.71650E-03	4.03052E+02	5.43E-09
OH-	OH-	1.19758E-06	8.31822E-07	0.6946	4.87380E-08	1.18133E-06	2.00912E-02	-1.85E-07
Am(CO3)3=	Am(CO3)3=	1.87813E-07	2.44036E-09	1.2994E-02	7.64348E-09	1.85265E-07	7.83721E-02	-2.49E-07
H+	H+	1.99837E-08	1.19307E-08	0.5970	8.13282E-10	1.97125E-08	1.98683E-05	1.87E-07
Am(CO3)2-	Am(CO3)2-	5.09341E-09	2.92780E-09	0.5748	2.07287E-10	5.02429E-09	1.82391E-03	2.15E-10
AmCO3+	AmCO3+	8.78026E-11	5.06082E-11	0.5764	3.57332E-12	8.66111E-11	2.62440E-05	1.92E-07
Am+++	Am+++	5.88554E-13	1.25606E-15	2.1341E-03	2.39525E-14	5.80567E-13	1.41078E-07	3.86E-07
AmOH++	(after_Cm(III))	3.16718E-16	3.07629E-17	9.0815E-02	1.28895E-17	3.12420E-16	8.12314E-11	2.00E-07
Am(OH)3(aq)	(1e-9m_minimum)	1.14525E-16	1.14525E-16	1.000	4.66083E-18	1.12971E-16	3.32158E-11	-1.74E-07
Am(OH)2+	(after_Cm(III))	3.00967E-17	1.73473E-17	0.5764	1.22485E-18	2.96882E-17	8.22408E-12	1.23E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.81637E-01	9.83896E-01	1.002	2.26555E+00	5.47055E+01	9.85530E+05	
NaAm(CO3)2.6H2O(c)		9.52851E+01	1.00000E+00	1.000	3.88900E+00	9.39064E+01	4.63991E+07	
Na+	Na+	5.19192E-01	3.12414E-01	0.6017	2.11905E-02	5.11680E-01	1.17634E+04	
HCO3-	HCO3-	5.04656E-01	2.99950E-01	0.5944	2.05972E-02	4.97354E-01	3.03471E+04	
CO2(aq)	CO2(aq)	7.26833E-03	8.06364E-03	1.109	2.96652E-04	7.16316E-03	3.15249E+02	
CO3=	CO3=	7.26888E-03	1.12930E-03	0.1554	2.96593E-04	7.16173E-03	4.29770E+02	3.87E-11
OH-	OH-	1.17699E-06	8.15267E-07	0.6927	4.80381E-08	1.15996E-06	1.97278E-02	-1.50E-08
Am(CO3)3=	Am(CO3)3=	2.01721E-07	2.40594E-09	1.1927E-02	8.23312E-09	1.98803E-07	8.40950E-02	-1.54E-08
H+	H+	2.05691E-08	1.21616E-08	0.5913	8.39513E-10	2.02715E-08	2.04316E-05	1.50E-08
Am(CO3)2-	Am(CO3)2-	4.92245E-09	2.79575E-09	0.5680	2.00907E-10	4.85123E-09	1.76108E-03	1.88E-11
AmCO3+	AmCO3+	8.21790E-11	4.68060E-11	0.5696	3.35408E-12	8.09899E-11	2.45407E-05	1.54E-08
Am+++	Am+++	6.09549E-13	1.12516E-15	1.8459E-03	2.48783E-14	6.00729E-13	1.45977E-07	3.11E-08
AmOH++	(after_Cm(III))	2.93489E-16	2.52526E-17	9.6043E-02	1.19786E-17	2.89243E-16	7.52052E-11	1.61E-08
Am(OH)3(aq)	(1e-9m_minimum)	9.65853E-17	9.65853E-17	1.000	3.94207E-18	9.51878E-17	2.79873E-11	-1.39E-08
Am(OH)2+	(after_Cm(III))	2.62080E-17	1.49271E-17	0.5696	1.06966E-18	2.58288E-17	7.15496E-12	1.02E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.80578E-01	9.82984E-01	1.002	2.27205E+00	5.46559E+01	9.84638E+05	
NaAm(CO3)2.6H2O(c)		9.50124E+01	1.00000E+00	1.000	3.88900E+00	9.35528E+01	4.62244E+07	
Na+	Na+	5.49731E-01	3.27930E-01	0.5965	2.25013E-02	5.41286E-01	1.24440E+04	
HCO3-	HCO3-	5.34280E-01	3.14654E-01	0.5889	2.18689E-02	5.26073E-01	3.20994E+04	
CO2(aq)	CO2(aq)	7.72568E-03	8.62354E-03	1.116	3.16223E-04	7.60699E-03	3.34782E+02	
CO3=	CO3=	7.72423E-03	1.16313E-03	0.1506	3.16164E-04	7.60557E-03	4.56404E+02	1.96E-11
OH-	OH-	1.15726E-06	7.99705E-07	0.6910	4.73685E-08	1.13949E-06	1.93796E-02	-1.34E-08
Am(CO3)3=	Am(CO3)3=	2.16127E-07	2.37394E-09	1.0984E-02	8.84640E-09	2.12807E-07	9.00232E-02	-1.37E-08
H+	H+	2.11419E-08	1.23867E-08	0.5859	8.65367E-10	2.08171E-08	2.09815E-05	1.33E-08
Am(CO3)2-	Am(CO3)2-	4.76987E-09	2.67833E-09	0.5615	1.95238E-10	4.69659E-09	1.70495E-03	1.64E-11
AmCO3+	AmCO3+	7.73083E-11	4.35362E-11	0.5632	3.16434E-12	7.61207E-11	2.30653E-05	1.37E-08
Am+++	Am+++	6.32222E-13	1.01612E-15	1.6072E-03	2.58778E-14	6.22510E-13	1.51270E-07	2.77E-08
AmOH++	(after_Cm(III))	2.73701E-16	2.23701E-17	8.1732E-02	1.12030E-17	2.69496E-16	7.00709E-11	1.43E-08
Am(OH)3(aq)	(1e-9m_minimum)	8.23253E-17	8.23253E-17	1.000	3.36969E-18	8.10606E-17	2.38336E-11	-1.24E-08
Am(OH)2+	(after_Cm(III))	2.30326E-17	1.29708E-17	0.5632	9.42759E-19	2.26787E-17	6.28234E-12	9.11E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.79527E-01	9.82079E-01	1.003	2.27855E+00	5.46068E+01	9.83752E+05	
NaAm(CO3)2.6H2O(c)		9.47413E+01	1.00000E+00	1.000	3.88900E+00	9.32020E+01	4.60510E+07	
Na+	Na+	5.80095E-01	3.43218E-01	0.5917	2.38121E-02	5.70670E-01	1.31196E+04	

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHC03_QB0204.OUT
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HCO3-	HCO3-	5.63732E-01	3.29128E-01	0.5838	2.31404E-02	5.54572E-01	3.38384E+04	
CO2 (aq)	CO2 (aq)	8.18235E-03	9.18891E-03	1.123	3.35874E-04	8.04940E-03	3.54252E+02	
CO3=	CO3=	8.18090E-03	1.19540E-03	0.1461	3.35815E-04	8.04798E-03	4.82953E+02	
OH-	OH-	1.13832E-06	7.85024E-07	0.6896	4.67263E-08	1.11982E-06	1.90451E+02	5.11E-12
Am(CO3)3=-	Am(CO3)3=-	2.31056E-07	2.34405E-09	1.0145E-02	9.48453E-09	2.27302E-07	9.61550E-02	-1.20E-08
H+	H+	2.17032E-08	1.26068E-08	0.5809	8.90886E-10	2.13506E-08	2.15192E-05	1.20E-08
Am(CO3)2-	Am(CO3)2-	4.63279E-09	2.57322E-09	0.5554	1.90170E-10	4.55752E-09	1.65446E-03	1.45E-11
AmCO3+	AmCO3+	7.30527E-11	4.06984E-11	0.5571	2.99871E-12	7.18657E-11	2.17760E-05	1.23E-08
Am+++	Am+++	6.56481E-13	9.24242E-16	1.4079E-03	2.68476E-14	6.45815E-13	1.56933E-07	2.49E-08
AmOH++	(after_Cm(III))	2.56669E-16	1.99738E-17	7.7819E-02	1.05359E-17	2.52499E-16	6.36515E-11	1.29E-08
Am(OH)3(aq)	(1e-9m_minimum)	7.08328E-17	7.08328E-17	1.000	2.90759E-18	6.96819E-17	2.04880E-11	-1.11E-08
Am(OH)2+	(after_Cm(III))	2.04067E-17	1.13688E-17	0.5571	8.37668E-19	2.00752E-17	5.56112E-12	8.25E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.78484E-01	9.81180E-01	1.003	2.28506E+00	5.45580E+01	9.82873E+05	
NaAm(CO3)2.6H2O(c)	Na+	9.44717E+01	1.00000E+00	1.000	3.88900E+00	9.28537E+01	4.58790E+07	
Na+	Na+	6.10287E-01	3.58291E-01	0.5871	2.51229E-02	5.99834E-01	1.37901E+04	
HCO3-	HCO3-	5.93011E-01	3.43386E-01	0.5791	2.44117E-02	5.82855E-01	3.55641E+04	
CO2(aq)	CO2(aq)	8.63829E-03	9.75970E-03	1.130	3.55601E-04	8.49033E-03	3.73658E+02	
CO3=	CO3=	8.63685E-03	1.22623E-03	0.1420	3.55542E-04	8.48892E-03	5.09413E+02	-5.86E-12
OH-	OH-	1.12008E-06	7.71131E-07	0.6885	4.61088E-08	1.10089E-06	1.87232E-02	-1.09E-08
Am(CO3)3=-	Am(CO3)3=-	2.46533E-07	2.31604E-09	9.3944E-03	1.01487E-08	2.42311E-07	1.02504E-01	-1.12E-08
H+	H+	2.22541E-08	1.28222E-08	0.5762	9.16105E-10	2.18729E-08	2.20457E-05	1.08E-08
Am(CO3)2-	Am(CO3)2-	4.50894E-09	2.47854E-09	0.5497	1.85614E-10	4.43171E-09	1.60879E-03	1.28E-11
AmCO3+	AmCO3+	6.93056E-11	3.82153E-11	0.5514	2.85302E-12	6.81186E-11	2.06406E-05	1.12E-08
Am+++	Am+++	6.82261E-13	8.46031E-16	1.2400E-03	2.80858E-14	6.70576E-13	1.62950E-07	2.26E-08
AmOH++	(after_Cm(III))	2.41878E-16	1.79600E-17	7.4252E-02	9.95710E-18	2.37736E-16	6.18130E-11	1.17E-08
Am(OH)3(aq)	(1e-9m_minimum)	6.14567E-17	6.14567E-17	1.000	2.52991E-18	6.04041E-17	1.77601E-11	-1.01E-08
Am(OH)2+	(after_Cm(III))	1.82111E-17	1.00416E-17	0.5514	7.49673E-19	1.78992E-17	4.95834E-12	7.52E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.77450E-01	9.80288E-01	1.003	2.29156E+00	5.45095E+01	9.82000E+05	
NaAm(CO3)2.6H2O(c)	Na+	9.42037E+01	1.00000E+00	1.000	3.88900E+00	9.25080E+01	4.57082E+07	
Na+	Na+	6.40307E-01	3.73161E-01	0.5828	2.64337E-02	6.28781E-01	1.44555E+04	
HCO3-	HCO3-	6.22121E-01	3.57438E-01	0.5745	2.56829E-02	6.10923E-01	3.72767E+04	
CO2(aq)	CO2(aq)	9.09346E-03	1.03358E-02	1.137	3.75404E-04	8.92978E-03	3.92998E+02	
CO3=	CO3=	9.09202E-03	1.25573E-03	0.1381	3.75345E-04	8.92836E-03	5.35784E+02	-1.43E-11
OH-	OH-	1.10249E-06	7.57945E-07	0.6875	4.55140E-08	1.08265E-06	1.84129E-02	-9.90E-09
Am(CO3)3=-	Am(CO3)3=-	2.62584E-07	2.28971E-09	8.7199E-03	1.08402E-08	2.57857E-07	1.09081E-01	-1.02E-08
H+	H+	2.27953E-08	1.30334E-08	0.5718	9.41057E-10	2.23850E-08	2.25619E-05	9.91E-09
Am(CO3)2-	Am(CO3)2-	4.39646E-09	2.39280E-09	0.5443	1.81499E-10	4.31733E-09	1.56727E-03	1.15E-11
AmCO3+	AmCO3+	6.59836E-11	3.60267E-11	0.5460	2.72399E-12	6.47959E-11	1.96339E-05	1.02E-08
Am+++	Am+++	7.09514E-13	7.78846E-16	1.0977E-03	2.92908E-14	6.96743E-13	1.69308E-07	2.06E-08
AmOH++	(after_Cm(III))	2.28931E-16	1.62510E-17	7.0987E-02	9.45091E-18	2.24810E-16	5.84522E-11	1.07E-08
Am(OH)3(aq)	(1e-9m_minimum)	5.37233E-17	5.37233E-17	1.000	2.21785E-18	5.27562E-17	1.55115E-11	-9.21E-09
Am(OH)2+	(after_Cm(III))	1.63569E-17	8.93076E-18	0.5460	6.75258E-19	1.60624E-17	4.44953E-12	6.92E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.76423E-01	9.79402E-01	1.003	2.29806E+00	5.44614E+01	9.81134E+05	
NaAm(CO3)2.6H2O(c)	Na+	9.39372E+01	1.00000E+00	1.000	3.88900E+00	9.21649E+01	4.55386E+07	
Na+	Na+	6.70157E-01	3.87837E-01	0.5787	2.77445E-02	6.57514E-01	4.51161E+04	
HCO3-	HCO3-	6.51063E-01	3.71295E-01	0.5703	2.69540E-02	6.38780E-01	3.89765E+04	
CO2(aq)	CO2(aq)	9.54783E-03	1.09173E-02	1.143	3.95280E-04	9.36770E-03	4.12270E+02	
CO3=	CO3=	9.54639E-03	1.28398E-03	0.1345	3.95221E-04	9.36629E-03	5.62063E+02	-2.08E-11
OH-	OH-	1.08551E-06	7.45397E-07	0.6867	4.49399E-08	1.06503E-06	1.81132E-02	-9.11E-09
Am(CO3)3=-	Am(CO3)3=-	2.79231E-07	2.26488E-09	8.1111E-03	1.15602E-08	2.73963E-07	1.15894E-01	-9.37E-09
H+	H+	2.33277E-08	1.32408E-08	0.5676	9.65768E-10	2.28876E-08	2.30684E-05	9.12E-09
Am(CO3)2-	Am(CO3)2-	4.29385E-09	2.31478E-09	0.5391	1.77765E-10	4.21284E-09	1.52934E-03	1.03E-11
AmCO3+	AmCO3+	6.30202E-11	3.40852E-11	0.5409	2.60904E-12	6.18313E-11	1.87354E-05	9.39E-09
Am+++	Am+++	7.38209E-13	7.20680E-16	9.7623E-04	3.05619E-14	7.24282E-13	1.76001E-07	1.90E-08
AmOH++	(after_Cm(III))	2.17515E-16	1.47881E-17	6.7986E-02	9.00512E-18	2.13411E-16	5.54885E-11	9.81E-09
Am(OH)3(aq)	(1e-9m_minimum)	4.72817E-17	4.72817E-17	1.000	1.95746E-18	4.63896E-17	1.36396E-11	-8.47E-09
Am(OH)2+	(after_Cm(III))	1.47769E-17	7.99224E-18	0.5409	6.11763E-19	1.44981E-17	4.01618E-12	6.41E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.75405E-01	9.78522E-01	1.003	2.30456E+00	5.44137E+01	9.80274E+05	
NaAm(CO3)2.6H2O(c)	Na+	9.36721E+01	1.00000E+00	1.000	3.88900E+00	9.18244E+01	4.53704E+07	
Na+	Na+	6.99839E-01	4.02330E-01	0.5749	2.90553E-02	6.86034E-01	1.57718E+04	
HCO3-	HCO3-	6.79837E-01	3.84967E-01	0.5663	2.82249E-02	6.66427E-01	4.06634E+04	
CO2(aq)	CO2(aq)	1.00014E-02	1.15039E-02	1.150	4.15228E-04	9.80408E-03	4.31475E+02	
CO3=	CO3=	9.99993E-03	1.31106E-03	0.1311	4.15168E-04	9.80267E-03	5.88250E+02	-2.59E-11
OH-	OH-	1.06908E-06	7.33431E-07	0.6860	4.43851E-08	1.04799E-06	1.78235E-02	-8.44E-09
Am(CO3)3=-	Am(CO3)3=-	2.96499E-07	2.24140E-09	7.5596E-03	1.23098E-08	2.90650E-07	1.22953E-01	-8.68E-09
H+	H+	2.38519E-08	1.34447E-08	0.5637	9.90262E-10	2.33814E-08	2.35661E-05	8.45E-09
Am(CO3)2-	Am(CO3)2-	4.19985E-09	2.24346E-09	0.5342	1.74366E-10	4.11700E-09	1.49455E-03	9.38E-12
AmCO3+	AmCO3+	6.03620E-11	3.23526E-11	0.5360	2.50606E-12	5.91713E-11	1.79295E-05	8.70E-09
Am+++	Am+++	7.68323E-13	6.69898E-16	8.7190E-04	3.18986E-14	7.53167E-13	1.83020E-07	1.76E-08
AmOH++	(after_Cm(III))	2.07385E-16	1.35257E-17	6.5220E-02	8.61004E-18	2.03294E-16	5.28580E-11	9.10E-09
Am(OH)3(aq)	(1e-9m_minimum)	4.18682E-17	4.18682E-17	1.000	1.73825E-18	4.10423E-17	1.20673E-11	-7.85E-09
Am(OH)2+	(after_Cm(III))	1.34197E-17	7.19265E-18	0.5360	5.57148E-19	1.31550E-17	3.64413E-12	5.98E-10

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHCO3_QB0204.OUT
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.74394E-01	9.77648E-01	1.003	2.31106E+00	5.43663E+01	9.79421E+05
NaAm(CO3)2.6H2O(c)		9.34086E+01	1.00000E+00	1.000	3.88900E+00	9.14863E+01	4.52033E+07
Na+	Na+	7.29354E-01	4.16647E-01	0.5713	3.03661E-02	7.14344E-01	1.64226E+04
HCO3-	HCO3-	7.08447E-01	3.98461E-01	0.5624	2.94957E-02	6.93868E-01	4.23378E+04
CO2(aq)	CO2(aq)	1.04540E-02	1.20958E-02	1.157	4.35246E-04	1.02389E-02	4.50612E+02
CO3=	CO3=	1.04526E-02	1.33705E-03	0.1279	4.35187E-04	1.02375E-02	6.14344E+02
OH-	OH-	1.05317E-06	7.21944E-07	0.6855	4.38480E-08	1.03150E-06	1.75430E-02
Am(CO3)3=-	Am(CO3)3=-	3.14412E-07	2.21916E-09	7.0581E-03	1.30903E-08	3.07942E-07	1.30268E-01
H+	H+	2.43684E-08	1.36455E-08	0.5600	1.01456E-09	2.38669E-08	2.40554E-05
Am(CO3)2-	Am(CO3)2-	4.11341E-09	2.17802E-09	0.5295	1.71259E-10	4.02876E-09	1.46251E-03
AmCO3+	AmCO3+	5.79656E-11	3.07983E-11	0.5313	2.41335E-12	5.67727E-11	1.72026E-05
Am+++	Am+++	1.98844E-13	6.25316E-16	7.8180E-04	3.33009E-14	7.83384E-13	1.90362E-07
AmOH++	(after Cm(III))	1.98345E-16	1.24287E-17	6.2662E-02	8.25793E-18	1.94263E-16	5.05097E-11
Am(OH)3(aq)	(1e-9m_minimum)	3.72820E-17	3.72820E-17	1.000	1.55221E-18	3.65148E-17	1.07361E-11
Am(OH)2+	(after Cm(III))	1.22454E-17	6.50622E-18	0.5313	5.09828E-19	1.19934E-17	3.32234E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.73391E-01	9.76779E-01	1.003	2.31757E+00	5.43193E+01	9.78573E+05
NaAm(CO3)2.6H2O(c)		9.31465E+01	1.00000E+00	1.000	3.88900E+00	9.11507E+01	4.50375E+07
Na+	Na+	7.58703E-01	4.30797E-01	0.5678	3.16769E-02	7.42447E-01	1.70687E+04
HCO3-	HCO3-	7.36893E-01	4.11787E-01	0.5588	3.07663E-02	7.21103E-01	4.39969E+04
CO2(aq)	CO2(aq)	1.09058E-02	1.26928E-02	1.164	4.55334E-04	1.06722E-02	4.69679E+02
CO3=	CO3=	1.09044E-02	1.36202E-03	0.1249	4.55274E-04	1.06707E-02	6.40343E+02
OH-	OH-	1.03775E-06	7.11044E-07	0.6852	4.33276E-08	1.01552E-06	1.72712E-02
Am(CO3)3=-	Am(CO3)3=-	3.32993E-07	2.19804E-09	6.6008E-03	1.39029E-08	3.25859E-07	1.37847E-01
H+	H+	2.48777E-08	1.38433E-08	0.5565	1.03868E-09	2.43447E-08	2.45370E-05
Am(CO3)2-	Am(CO3)2-	4.03366E-09	2.11774E-09	0.5250	1.68411E-10	3.94723E-09	1.43292E-03
AmCO3+	AmCO3+	5.57952E-11	2.93970E-11	0.5269	2.32953E-12	5.45997E-11	1.65442E-05
Am+++	Am+++	8.32765E-13	5.85923E-16	7.0359E-04	3.47691E-14	8.14921E-13	1.98026E-07
AmOH++	(after Cm(III))	1.90233E-16	1.14691E-17	6.0290E-02	7.94251E-18	1.86157E-16	4.84022E-11
Am(OH)3(aq)	(1e-9m_minimum)	3.33678E-17	3.33678E-17	1.000	1.39315E-18	3.26529E-17	9.60067E-12
Am(OH)2+	(after Cm(III))	1.12225E-17	5.91283E-18	0.5269	4.68555E-19	1.09820E-17	3.04218E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.72396E-01	9.75917E-01	1.004	2.32407E+00	5.42726E+01	9.77732E+05
NaAm(CO3)2.6H2O(c)		9.28859E+01	1.00000E+00	1.000	3.88900E+00	9.08176E+01	4.48729E+07
Na+	Na+	7.87888E-01	4.44787E-01	0.5645	3.29877E-02	7.70344E-01	1.77100E+04
HCO3-	HCO3-	7.65176E-01	4.24951E-01	0.5554	3.20368E-02	7.48137E-01	4.56492E+04
CO2(aq)	CO2(aq)	1.13567E-02	1.32950E-02	1.171	4.75489E-04	1.11038E-02	4.88677E+02
CO3=	CO3=	1.13553E-02	1.38602E-03	0.1221	4.75429E-04	1.11024E-02	6.66247E+02
OH-	OH-	1.02279E-06	7.00541E-07	0.6849	4.28226E-08	1.00001E-06	1.70075E-02
Am(CO3)3=-	Am(CO3)3=-	3.52267E-07	2.17794E-09	6.1826E-03	1.47489E-08	3.44423E-07	1.45701E-01
H+	H+	2.53803E-08	1.40385E-08	0.5531	1.06264E-09	2.48152E-08	2.50112E-05
Am(CO3)2-	Am(CO3)2-	3.95984E-09	2.06204E-09	0.5207	1.65793E-10	3.87166E-09	1.40549E-03
AmCO3+	AmCO3+	5.38213E-11	2.81280E-11	0.5226	2.25342E-12	5.26228E-11	1.59452E-05
Am+++	Am+++	8.67084E-13	5.90922E-16	6.3537E-04	3.63035E-14	8.47776E-13	2.06010E-07
AmOH++	(after Cm(III))	1.82921E-16	1.06247E-17	5.8084E-02	7.65864E-18	1.78848E-16	4.65017E-11
Am(OH)3(aq)	(1e-9m_minimum)	3.00047E-17	3.00047E-17	1.000	1.25625E-18	2.93366E-17	8.62560E-12
Am(OH)2+	(after Cm(III))	1.03260E-17	5.39659E-18	0.5226	4.32337E-19	1.00961E-17	2.79677E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.71408E-01	9.75059E-01	1.004	2.33057E+00	5.42263E+01	9.76898E+05
NaAm(CO3)2.6H2O(c)		9.26257E+01	1.00000E+00	1.000	3.88900E+00	9.04869E+01	4.47095E+07
Na+	Na+	8.16910E-01	4.58622E-01	0.5614	3.42986E-02	7.98038E-01	1.83467E+04
HCO3-	HCO3-	7.93298E-01	4.37960E-01	0.5521	3.33072E-02	7.74971E-01	4.72865E+04
CO2(aq)	CO2(aq)	1.18067E-02	1.39022E-02	1.177	4.95711E-04	1.15396E-02	5.07605E+02
CO3=	CO3=	1.18052E-02	1.40912E-03	0.1194	4.95651E-04	1.15325E-02	6.92056E+02
OH-	OH-	1.00825E-06	6.90451E-07	0.6848	4.23321E-08	9.84957E-07	1.67515E-02
Am(CO3)3=-	Am(CO3)3=-	3.72257E-07	2.15878E-09	5.7992E-03	1.56295E-08	3.63657E-07	1.53837E-01
H+	H+	2.58767E-08	1.42311E-08	0.5500	1.08645E-09	2.52789E-08	2.54786E-05
Am(CO3)2-	Am(CO3)2-	3.89133E-09	2.01040E-09	0.5166	1.63380E-10	3.80143E-09	1.37999E-03
AmCO3+	AmCO3+	5.20192E-11	2.69743E-11	0.5185	2.18406E-12	5.08174E-11	1.53981E-05
Am+++	Am+++	9.02805E-13	5.19666E-16	5.7561E-04	3.79049E-14	8.81948E-13	2.14313E-07
AmOH++	(after Cm(III))	1.76300E-16	9.87756E-18	5.6027E-02	7.40208E-18	1.72227E-16	4.47803E-11
Am(OH)3(aq)	(1e-9m_minimum)	2.70970E-17	2.70970E-17	1.000	1.13769E-18	2.64710E-17	7.78306E-12
Am(OH)2+	(after Cm(III))	9.53600E-18	4.94484E-18	0.5185	4.00376E-19	9.31570E-18	2.58058E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.70428E-01	9.74208E-01	1.004	2.33707E+00	5.41803E+01	9.76069E+05
NaAm(CO3)2.6H2O(c)		9.23690E+01	1.00000E+00	1.000	3.88900E+00	9.01585E+01	4.45473E+07
Na+	Na+	8.45771E-01	4.72310E-01	0.5584	3.56094E-02	8.25531E-01	1.89788E+04
HCO3-	HCO3-	8.21260E-01	4.50819E-01	0.5489	3.45774E-02	8.01607E-01	4.89117E+04
CO2(aq)	CO2(aq)	1.22557E-02	1.45144E-02	1.184	5.15999E-04	1.19624E-02	5.26463E+02
CO3=	CO3=	1.22542E-02	1.43135E-03	0.1168	5.15938E-04	1.19610E-02	6.17769E+02
OH-	OH-	9.94119E-07	6.80745E-07	0.6848	4.18552E-08	9.70329E-07	1.65027E-02
Am(CO3)3=-	Am(CO3)3=-	3.92987E-07	2.14049E-09	5.4467E-03	1.65459E-08	3.83582E-07	1.62266E-01
H+	H+	2.63670E-08	1.44214E-08	0.5469	1.11013E-09	2.57361E-08	2.59394E-05
Am(CO3)2-	Am(CO3)2-	3.82757E-09	1.96241E-09	0.5127	1.61151E-10	3.73597E-09	1.35623E-03

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHC03_QB0204.OUT
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AmCO3+	AmCO3+	5.03682E-11	2.59212E-11	0.5146	2.12064E-12	4.91628E-11	1.48968E-05	1.09E-08
Am+++	Am+++	9.39934E-13	4.91622E-16	5.2304E-04	3.95739E-14	9.17440E-13	2.22938E-07	2.21E-08
AmOH++	(after_Cm(III))	1.70281E-16	9.21315E-18	5.4105E-02	7.16932E-18	1.66206E-16	4.32148E-11	1.14E-08
Am(OH)3(aq)	(1e-9m_minimum)	2.45687E-17	2.45687E-17	1.000	1.03441E-18	2.39808E-17	7.05088E-12	-9.82E-09
Am(OH)2+	(after_Cm(III))	8.83614E-18	4.54739E-18	0.5146	3.72027E-19	8.62468E-18	2.38916E-12	7.73E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.69455E-01	9.73361E-01	1.004	2.34358E+00	5.41346E+01	9.75246E+05
NaAm(CO3)2.6H2O(c)	Na+	9.21127E+01	1.00000E+00	1.000	3.88900E+00	8.98326E+01	4.43862E+07
Na+	Na+	8.74471E-01	4.85855E-01	0.5556	3.69202E-02	8.52825E-01	1.96062E+04
HCO3-	HCO3-	8.49065E-01	4.63535E-01	0.5459	3.58475E-02	8.28047E-01	5.05250E+04
CO2(aq)	CO2(aq)	1.27037E-02	1.51317E-02	1.191	5.36352E-04	1.23893E-02	5.45250E+02
CO3=	CO3=	1.27023E-02	1.45277E-03	0.1144	5.36290E-04	1.23879E-02	7.43385E+02
OH-	OH-	9.80372E-07	6.71395E-07	0.6848	4.13913E-08	9.56104E-07	1.62607E-02
Am(CO3)3=-	Am(CO3)3=-	4.14481E-07	2.12300E-09	5.1221E-03	1.74994E-08	4.04221E-07	1.70996E-01
H+	H+	2.68518E-08	1.46095E-08	0.5441	1.13368E-09	2.61871E-08	2.63940E-05
Am(CO3)2-	Am(CO3)2-	3.76809E-09	1.91767E-09	0.5089	1.59089E-10	3.67482E-09	1.33403E-03
AmCO3+	AmCO3+	4.88507E-11	2.49568E-11	0.5109	2.06247E-12	4.76414E-11	1.44358E-05
Am+++	Am+++	9.78481E-13	4.66352E-16	4.7661E-04	4.13115E-14	9.54260E-13	2.31885E-07
AmOH++	(after_Cm(III))	1.64789E-16	8.61954E-18	5.2306E-02	6.95740E-18	1.60710E-16	4.17858E-11
Am(OH)3(aq)	(1e-9m_minimum)	2.23587E-17	2.23587E-17	1.000	9.43983E-19	2.18052E-17	6.41121E-12
Am(OH)2+	(after_Cm(III))	8.21320E-18	4.19596E-18	0.5109	3.46761E-19	8.00989E-18	2.21886E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.68489E-01	9.72520E-01	1.004	2.35008E+00	5.40893E+01	9.74429E+05
NaAm(CO3)2.6H2O(c)	Na+	9.18579E+01	1.00000E+00	1.000	3.88900E+00	8.95090E+01	4.42253E+07
Na+	Na+	9.03013E-01	4.99263E-01	0.5529	3.23108E-02	8.79922E-01	2.02292E+04
HCO3-	HCO3-	8.76712E-01	4.76113E-01	0.5431	3.71175E-02	8.54294E-01	5.21255E+04
CO2(aq)	CO2(aq)	1.31508E-02	1.57539E-02	1.198	5.56768E-04	1.28145E-02	5.63966E+02
CO3=	CO3=	1.31494E-02	1.47342E-03	0.1121	5.56706E-04	1.28131E-02	7.68905E+02
OH-	OH-	9.66988E-07	6.62377E-07	0.6850	4.09395E-08	9.42261E-07	1.60253E-02
Am(CO3)3=-	Am(CO3)3=-	4.36762E-07	2.10625E-09	4.8224E-03	1.84912E-08	4.25594E-07	1.80038E-01
H+	H+	2.73312E-08	1.47956E-08	0.5413	1.15713E-09	2.66323E-08	2.68427E-05
Am(CO3)2-	Am(CO3)2-	3.71248E-09	1.87588E-09	0.5053	1.57176E-10	3.61755E-09	1.31324E-03
AmCO3+	AmCO3+	4.74517E-11	2.40580E-11	0.5073	2.00897E-12	4.62383E-11	1.40106E-05
Am+++	Am+++	1.01846E-12	4.43409E-16	4.3545E-04	4.31186E-14	9.92415E-13	2.41157E-07
AmOH++	(after_Cm(III))	1.59761E-16	8.08688E-18	5.0619E-02	6.76383E-18	1.55676E-16	4.04769E-11
Am(OH)3(aq)	(1e-9m_minimum)	2.04173E-17	2.04173E-17	1.000	8.64408E-19	1.98952E-17	5.84962E-12
Am(OH)2+	(after_Cm(III))	7.65628E-18	3.88379E-18	0.5073	3.24145E-19	7.46050E-18	2.06667E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.67531E-01	9.71684E-01	1.004	2.35658E+00	5.40443E+01	9.73618E+05
NaAm(CO3)2.6H2O(c)	Na+	9.16044E+01	1.00000E+00	1.000	3.88900E+00	8.91877E+01	4.40676E+07
Na+	Na+	9.31397E-01	5.12539E-01	0.5503	3.95418E-02	9.06825E-01	2.08477E+04
HCO3-	HCO3-	9.04204E-01	4.88558E-01	0.5403	3.83873E-02	8.80349E-01	5.37164E+04
CO2(aq)	CO2(aq)	1.35969E-02	1.63810E-02	1.205	5.77247E-04	1.32382E-02	5.82610E+02
CO3=	CO3=	1.35954E-02	1.49335E-03	0.1098	5.77184E-04	1.32368E-02	7.94327E+02
OH-	OH-	9.53950E-07	6.53670E-07	0.6852	4.04992E-08	9.28783E-07	1.57961E-02
Am(CO3)3=-	Am(CO3)3=-	4.59855E-07	2.09019E-09	4.5453E-03	1.95228E-08	4.47724E-07	1.89399E-01
H+	H+	2.78056E-08	1.49798E-08	0.5387	1.18047E-09	2.70720E-08	2.72859E-05
Am(CO3)2-	Am(CO3)2-	3.66039E-09	1.83674E-09	0.5018	1.55399E-10	3.56382E-09	1.29373E-03
AmCO3+	AmCO3+	4.61583E-11	2.32542E-11	0.5038	1.95962E-12	4.49406E-11	1.36174E-05
Am+++	Am+++	1.05988E-12	4.22729E-16	3.9885E-04	4.49963E-14	1.03192E-12	2.50755E-07
AmOH++	(after_Cm(III))	1.55143E-16	7.60699E-18	4.9032E-02	6.58650E-18	1.51050E-16	3.92742E-11
Am(OH)3(aq)	(1e-9m_minimum)	1.87040E-17	1.87040E-17	1.000	7.94067E-19	1.82106E-17	5.35432E-12
Am(OH)2+	(after_Cm(III))	7.15632E-18	3.60530E-18	0.5038	3.03816E-19	6.96752E-18	1.93011E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.66580E-01	9.70853E-01	1.004	2.36308E+00	5.39996E+01	9.72813E+05
NaAm(CO3)2.6H2O(c)	Na+	9.13523E+01	1.00000E+00	1.000	3.88900E+00	8.88688E+01	4.39100E+07
Na+	Na+	9.59625E-01	5.25688E-01	0.5478	4.08526E-02	9.33536E-01	2.14618E+04
HCO3-	HCO3-	9.31541E-01	5.08974E-01	0.5377	3.96570E-02	9.06216E-01	5.52947E+04
CO2(aq)	CO2(aq)	1.40420E-02	1.70130E-02	1.212	5.97787E-04	1.36602E-02	6.01184E+02
CO3=	CO3=	1.40405E-02	1.51257E-03	0.1077	5.97724E-04	1.36588E-02	8.19653E+02
OH-	OH-	9.41241E-07	6.45253E-07	0.6855	4.00700E-08	9.15651E-07	1.55728E-02
Am(CO3)3=-	Am(CO3)3=-	4.83785E-07	2.07478E-09	4.2886E-03	2.05954E-08	4.70633E-07	1.99091E-01
H+	H+	2.82751E-08	1.51622E-08	0.5362	1.20371E-09	2.75064E-08	2.77237E-05
Am(CO3)2-	Am(CO3)2-	3.61148E-09	1.80002E-09	0.4984	1.53746E-10	3.51330E-09	1.27539E-03
AmCO3+	AmCO3+	4.49595E-11	2.24995E-11	0.5004	1.91399E-12	4.37372E-11	1.32528E-05
Am+++	Am+++	1.10275E-12	4.03812E-16	3.6618E-04	4.69458E-14	1.07277E-12	2.60684E-07
AmOH++	(after_Cm(III))	1.50890E-16	7.17302E-18	4.7538E-02	6.42358E-18	1.46787E-16	3.81658E-11
Am(OH)3(aq)	(1e-9m_minimum)	1.71858E-17	1.71858E-17	1.000	7.31622E-19	1.67185E-17	4.91562E-12
Am(OH)2+	(after_Cm(III))	6.70578E-18	3.35585E-18	0.5004	2.85475E-19	6.52347E-18	1.80710E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.65636E-01	9.70027E-01	1.005	2.36959E+00	5.39552E+01	9.72014E+05
NaAm(CO3)2.6H2O(c)	Na+	9.11016E+01	1.00000E+00	1.000	3.88900E+00	8.85520E+01	4.37535E+07
Na+	Na+	9.87698E-01	5.38713E-01	0.5454	4.21634E-02	9.60056E-01	2.20715E+04

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHC03_QB0204.OUT
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Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.64699E-01	9.69205E-01	1.005	2.37609E+00	5.39111E+01	9.71220E+05	
NaAm(CO3)2.6H2O(c)	9.08523E+01	1.00000E+00	1.000	3.88900E+00	8.82376E+01	4.35981E+07	
Na+	1.01562E+00	5.51618E-01	0.5431	4.34742E-02	9.86387E-01	2.26768E+04	
HCO3-	9.85759E-01	5.25137E-01	0.5327	4.21961E-02	9.57389E-01	5.84171E+04	
CO2(aq)	1.49291E-02	1.82915E-02	1.225	6.39050E-04	1.44994E-02	6.38116E+02	
CO3=	1.49276E-02	1.54908E-03	0.1038	6.38985E-04	1.44979E-02	8.70010E+02	1.16E-09
OH-	9.16751E-07	6.29226E-07	0.6864	3.92422E-08	8.90367E-07	1.51427E-02	-1.64E-07
Am(CO3)3--	5.34253E-07	2.04571E-09	3.8291E-03	2.28691E-08	5.18877E-07	2.19499E-01	-1.67E-07
H+	2.92005E-08	1.55219E-08	0.5316	1.24995E-09	2.83601E-08	2.85842E-05	1.63E-07
Am(CO3)2-	3.52219E-09	1.73297E-09	0.4941	1.83245E-10	4.15764E-11	1.24182E-03	1.52E-10
AmCO3+	4.28085E-11	2.11510E-11	0.4941	5.10651E-14	1.15862E-12	2.81544E-07	3.40E-07
Am+++	1.19295E-12	3.70662E-16	3.1071E-04	5.10651E-14	1.15862E-12	3.61925E-11	1.76E-07
AmOH++	1.43323E-16	6.42062E-18	4.4798E-02	6.13504E-18	1.39198E-16	3.61925E-11	1.76E-07
Am(OH)3(aq)	1.46284E-17	1.46284E-17	1.000	6.26179E-19	1.42074E-17	4.17728E-12	-1.50E-07
Am(OH)2+	5.92860E-18	2.92923E-18	0.4941	2.53778E-19	5.75798E-18	1.59504E-12	1.24E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.63769E-01	9.68389E-01	1.005	2.38259E+00	5.38674E+01	9.70432E+05	
NaAm(CO3)2.6H2O(c)	9.06043E+01	1.00000E+00	1.000	3.88900E+00	8.79254E+01	4.34439E+07	
Na+	1.04338E+00	5.64408E-01	0.5409	4.47850E-02	1.01253E+00	2.32779E+04	
HCO3-	1.01264E+00	5.37092E-01	0.5304	4.34655E-02	9.82700E-01	5.99615E+04	
CO2(aq)	1.53711E-02	1.89379E-02	1.232	6.59770E-04	1.49166E-02	6.56475E+02	
CO3=	1.53695E-02	1.56642E-03	0.1019	6.59704E-04	1.49151E-02	8.95042E+02	7.41E-11
OH-	9.04943E-07	6.21584E-07	0.6869	3.88428E-08	8.78186E-07	1.49356E-02	-7.81E-08
Am(CO3)3--	5.60840E-07	2.03199E-09	3.6231E-03	2.40729E-08	5.44257E-07	2.30236E-01	-8.03E-08
H+	2.96568E-08	1.56997E-08	0.5294	1.27296E-09	2.87799E-08	2.90073E-05	7.84E-08
Am(CO3)2-	3.48133E-09	1.70229E-09	0.4890	1.49429E-10	3.37839E-09	1.22642E-03	7.04E-11
AmCO3+	4.18405E-11	2.05465E-11	0.4911	1.79592E-12	4.06034E-11	1.23032E-05	8.09E-08
Am+++	1.24031E-12	3.56081E-16	2.8709E-04	5.32375E-14	1.20363E-12	2.92483E-07	1.64E-07
AmOH++	1.39946E-16	6.09315E-18	4.3539E-02	6.00689E-18	1.35808E-16	3.53111E-11	8.50E-08
Am(OH)3(aq)	1.35471E-17	1.35471E-17	1.000	5.81482E-19	1.31466E-17	3.86538E-12	-7.24E-08
Am(OH)2+	5.9205E-18	2.74607E-18	0.4911	2.40027E-19	5.42671E-18	1.50328E-12	5.99E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.62845E-01	9.67577E-01	1.005	2.38909E+00	5.38240E+01	9.69650E+05	
NaAm(CO3)2.6H2O(c)	9.03577E+01	1.00000E+00	1.000	3.88900E+00	8.76153E+01	4.32907E+07	
Na+	1.07100E+00	5.77085E-01	0.5388	4.60958E-02	1.03849E+00	2.38747E+04	
HCO3-	1.03938E+00	5.48933E-01	0.5281	4.47347E-02	1.00783E+00	6.14949E+04	
CO2(aq)	1.58120E-02	1.95890E-02	1.239	6.80548E-04	1.53321E-02	6.74762E+02	
CO3=	1.58104E-02	1.58320E-03	0.1001	6.80482E-04	1.53306E-02	9.19976E+02	-7.85E-11
OH-	8.93411E-07	6.14172E-07	0.6874	3.84524E-08	8.66296E-07	1.47334E-02	-4.17E-08
Am(CO3)3--	5.88363E-07	2.01876E-09	3.4311E-03	2.53231E-08	5.70506E-07	2.41340E-01	-4.31E-08
H+	3.01090E-08	1.58758E-08	0.5273	1.29589E-09	2.91952E-08	2.94259E-05	4.20E-08
Am(CO3)2-	3.44273E-09	1.67329E-09	0.4860	1.48175E-10	3.33824E-09	1.21184E-03	3.67E-11
AmCO3+	4.09355E-11	1.99825E-11	0.4881	1.76187E-12	3.96931E-11	1.20274E-05	4.33E-08
Am+++	1.28919E-12	3.42639E-16	2.6578E-04	5.54869E-14	1.25007E-12	3.03766E-07	8.80E-08
AmOH++	1.36805E-16	5.79321E-18	4.2346E-02	5.88810E-18	1.32653E-16	3.44908E-11	4.56E-08
Am(OH)3(aq)	1.25749E-17	1.25749E-17	1.000	5.41224E-19	1.21933E-17	3.58508E-12	-3.88E-08
Am(OH)2+	5.28480E-18	2.57976E-18	0.4881	2.27458E-19	5.12441E-18	1.41954E-12	3.22E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.61929E-01	9.66770E-01	1.005	2.39560E+00	5.37808E+01	9.68873E+05	
NaAm(CO3)2.6H2O(c)	9.01124E+01	1.00000E+00	1.000	3.88900E+00	8.73075E+01	4.31386E+07	
Na+	1.09846E+00	5.89653E-01	0.5368	4.74066E-02	1.06427E+00	2.44674E+04	
HCO3-	1.06596E+00	5.60665E-01	0.5260	4.60039E-02	1.03278E+00	6.30173E+04	
CO2(aq)	1.62518E-02	2.02448E-02	1.246	7.01384E-04	1.57460E-02	6.92977E+02	
CO3=	1.62503E-02	1.59942E-03	9.8424E-02	7.01317E-04	1.57445E-02	9.44812E+02	-8.44E-11
OH-	8.82143E-07	6.06977E-07	0.6881	3.80708E-08	8.54684E-07	1.45359E-02	-2.37E-08
Am(CO3)3--	6.16847E-07	2.00600E-09	3.2520E-03	2.66214E-08	5.97646E-07	2.52821E-01	-2.45E-08
H+	3.05574E-08	1.60506E-08	0.5253	1.31877E-09	2.96062E-08	2.98401E-05	2.39E-08
Am(CO3)2-	3.40621E-09	1.64585E-09	0.4832	1.47002E-10	3.30018E-09	1.19803E-03	2.04E-11
AmCO3+	4.00877E-11	1.94553E-11	0.4853	1.73007E-12	3.88399E-11	1.17688E-05	2.47E-08
Am+++	1.33963E-12	3.30215E-16	2.6450E-04	5.78147E-14	1.29793E-12	3.15397E-07	5.01E-08
AmOH++	1.33878E-16	5.51774E-18	4.1215E-02	5.77778E-18	1.29710E-16	3.3725E-11	2.59E-08
Am(OH)3(aq)	1.16980E-17	1.16980E-17	1.000	5.04852E-19	1.13339E-17	3.3240E-12	-2.21E-08
Am(OH)2+	5.00352E-18	2.42830E-18	0.4853	2.15938E-19	4.84777E-18	1.34290E-12	1.84E-09

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHC03_QB0204.OUT
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.61019E-01	9.65967E-01	1.005	2.40210E+00	5.37380E+01	9.68101E+05	
NaAm(CO3)2.6H2O(c)		8.98685E+01	1.00000E+00	1.000	3.88900E+00	8.70018E+01	4.29875E+07	
Na+	Na+	1.12578E+00	6.02116E-01	0.5348	4.87174E-02	1.08987E+00	2.50559E+04	
HCO3-	HCO3-	1.09240E+00	5.72291E-01	0.5239	4.72729E-02	1.05755E+00	6.45289E+04	
CO2(aq)	CO2(aq)	1.66906E-02	2.09053E-02	1.253	7.22276E-04	1.61582E-02	7.11120E+02	
CO3=	CO3=	1.66891E-02	1.61513E-03	9.6778E-02	7.22208E-04	1.61567E-02	9.69550E+02	-6.88E-11
OH-	OH-	8.71129E-07	5.99888E-07	0.6887	3.76975E-08	8.43341E-07	1.43430E-02	-1.40E-08
Am(CO3)3=-	Am(CO3)3=-	6.46318E-07	1.99368E-09	3.0847E-03	2.79690E-08	6.25701E-07	2.64689E-01	-1.44E-08
H+	H+	3.10019E-08	1.62241E-08	0.5233	1.34159E-09	3.00130E-08	3.02501E-05	1.41E-08
Am(CO3)2-	Am(CO3)2-	3.37162E-09	1.61983E-09	0.4804	1.45904E-10	3.26407E-09	1.18492E-03	1.18E-11
AmCO3+	AmCO3+	3.92922E-11	1.89616E-11	0.4826	1.70034E-12	3.80388E-11	1.15261E-05	1.45E-08
Am+++	Am+++	1.39164E-12	3.18705E-16	2.2901E-04	6.02224E-14	1.34725E-12	3.27382E-07	2.95E-08
AmOH++	(after_Cm(III))	1.31143E-16	5.26410E-18	4.0140E-02	5.67514E-18	1.26960E-16	3.30105E-11	1.53E-08
Am(OH)3(aq)	(1e-9m_minimum)	1.09047E-17	1.09047E-17	1.000	4.71895E-19	1.05569E-17	3.10395E-12	-1.30E-08
Am(OH)2+	(after_Cm(III))	4.74533E-18	2.29000E-18	0.4826	2.05351E-19	4.59396E-18	1.27259E-12	1.09E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.60116E-01	9.65170E-01	1.005	2.40860E+00	5.36955E+01	9.67335E+05	
NaAm(CO3)2.6H2O(c)		8.96259E+01	1.00000E+00	1.000	3.88900E+00	8.66982E+01	4.28375E+07	
Na+	Na+	1.15295E+00	6.14475E-01	0.5330	5.00282E-02	1.11529E+00	2.56403E+04	
HCO3-	HCO3-	1.11869E+00	5.83813E-01	0.5219	4.85418E-02	1.08215E+00	6.60298E+04	
CO2(aq)	CO2(aq)	1.71283E-02	2.15704E-02	1.259	7.43224E-04	1.65688E-02	7.29191E+02	
CO3=	CO3=	8.60360E-07	1.63034E-03	9.5193E-02	7.43154E-04	1.65673E-02	9.94190E+02	-5.44E-11
OH-	OH-	6.76801E-07	5.93195E-07	0.6895	3.73323E-08	8.32256E-07	1.41544E-02	-8.39E-09
Am(CO3)3=-	Am(CO3)3=-	3.14429E-08	1.63963E-08	2.9282E-03	2.93674E-08	6.54693E-07	2.76953E-01	-8.69E-09
H+	H+	3.33881E-09	1.59514E-09	0.4778	1.44876E-10	3.22975E-09	3.06561E-05	8.48E-09
Am(CO3)2-	Am(CO3)2-	3.85444E-11	1.84984E-11	0.4799	1.67250E-12	3.72853E-11	1.12724E-03	7.02E-12
AmCO3+	AmCO3+	1.44525E-12	3.08018E-16	2.1313E-04	6.27113E-14	1.39804E-12	3.39723E-07	1.78E-08
AmOH++	(after_Cm(III))	1.28585E-16	5.02998E-18	3.9118E-02	5.57949E-18	1.24385E-16	3.23409E-11	9.20E-09
Am(OH)3(aq)	(1e-9m_minimum)	1.01851E-17	1.01851E-17	1.000	4.41948E-19	9.85244E-18	2.8963E-12	-7.82E-09
Am(OH)2+	(after_Cm(III))	4.50776E-18	2.16338E-18	0.4799	1.95599E-19	4.36052E-18	1.20793E-12	6.57E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.59219E-01	9.64376E-01	1.005	2.41511E+00	5.36532E+01	9.66574E+05	
NaAm(CO3)2.6H2O(c)		8.93845E+01	1.00000E+00	1.000	3.88900E+00	8.63967E+01	4.26866E+07	
Na+	Na+	1.17997E+00	6.26735E-01	0.5311	5.13391E-02	1.14053E+00	2.62206E+04	
HCO3-	HCO3-	1.14484E+00	5.95234E-01	0.5199	4.98106E-02	1.06588E+00	6.75201E+04	
CO2(aq)	CO2(aq)	1.75649E-02	2.22401E-02	1.266	7.64226E-04	1.69778E-02	7.47190E+02	
CO3=	CO3=	1.75633E-02	1.64507E-03	9.3665E-02	7.64156E-04	1.69762E-02	1.01873E+03	-4.33E-11
OH-	OH-	8.49825E-07	5.86588E-07	0.6902	3.69747E-08	8.21419E-07	1.39701E-02	-4.70E-09
Am(CO3)3=-	Am(CO3)3=-	7.08323E-07	1.97027E-09	2.7816E-03	3.08182E-08	6.84647E-07	2.89625E-01	-4.87E-09
H+	H+	3.18803E-08	1.65674E-08	0.5197	1.38707E-09	3.08147E-08	3.10581E-05	4.74E-09
Am(CO3)2-	Am(CO3)2-	3.30767E-09	1.57167E-09	0.4752	1.43912E-10	3.19710E-09	1.16061E-03	3.88E-12
AmCO3+	AmCO3+	3.78404E-11	1.80630E-11	0.4773	1.64639E-12	3.65756E-11	1.10827E-05	4.89E-09
Am+++	Am+++	1.50047E-12	2.98075E-16	1.9866E-04	6.52832E-14	1.45031E-12	3.52426E-07	9.93E-09
AmOH++	(after_Cm(III))	1.26187E-16	4.81340E-18	3.8145E-02	5.49023E-18	1.21969E-16	3.17129E-11	5.15E-09
Am(OH)3(aq)	(1e-9m_minimum)	9.53068E-18	9.53068E-18	1.000	4.14667E-19	9.21210E-18	2.70856E-12	-4.37E-09
Am(OH)2+	(after_Cm(III))	4.28865E-18	2.04717E-18	0.4773	1.86593E-19	4.14529E-18	1.14831E-12	3.68E-10

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.58329E-01	9.63587E-01	1.005	2.42161E+00	5.36113E+01	9.65818E+05	
NaAm(CO3)2.6H2O(c)		8.91445E+01	1.00000E+00	1.000	3.88900E+00	8.60974E+01	4.25407E+07	
Na+	Na+	1.20685E+00	6.38987E-01	0.5294	5.26499E-02	1.16560E+00	2.67969E+04	
HCO3-	HCO3-	1.17085E+00	6.06558E-01	0.5180	5.10793E-02	1.13083E+00	6.89999E+04	
CO2(aq)	CO2(aq)	1.80004E-02	2.29144E-02	1.273	7.85283E-04	1.73851E-02	7.65116E+02	
CO3=	CO3=	1.79898E-02	1.65935E-03	9.2192E-02	7.85211E-04	1.73836E-02	1.04317E+03	-7.03E-11
OH-	OH-	8.39518E-07	5.80158E-07	0.6911	3.66246E-08	8.10822E-07	1.37899E-02	-1.30E-08
Am(CO3)3=-	Am(CO3)3=-	7.40911E-07	1.95914E-09	2.6442E-03	3.2228E-08	7.15585E-07	3.02712E-01	-1.35E-08
H+	H+	3.23144E-08	1.67373E-08	0.5180	1.40574E-09	3.12098E-08	3.14564E-05	1.32E-08
Am(CO3)2-	Am(CO3)2-	3.27806E-09	1.54935E-09	0.4726	1.43008E-10	3.16601E-09	1.14932E-03	1.04E-11
AmCO3+	AmCO3+	3.71768E-11	1.76532E-11	0.4748	1.62187E-12	3.59060E-11	1.08799E-05	1.36E-08
Am+++	Am+++	1.55732E-12	2.88806E-16	1.8545E-04	6.79395E-14	1.50409E-12	3.65494E-07	2.76E-08
AmOH++	(after_Cm(III))	1.23936E-16	4.61259E-18	3.7218E-02	5.40681E-18	1.19700E-16	3.11228E-11	1.43E-08
Am(OH)3(aq)	(1e-9m_minimum)	8.93396E-18	8.93396E-18	1.000	3.89751E-19	8.62858E-18	2.53699E-12	-1.21E-08
Am(OH)2+	(after_Cm(III))	4.08610E-18	1.94027E-18	0.4748	1.78260E-19	3.94643E-18	1.09322E-12	1.03E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.57855E-01	9.63166E-01	1.006	2.42810E+00	5.35890E+01	9.65416E+05	
NaAm(CO3)2.6H2O(c)		8.89060E+01	1.00000E+00	1.000	3.88900E+00	8.58313E+01	4.24092E+07	
Na+	Na+	1.22119E+00	6.45371E-01	0.5285	5.34182E-02	1.17895E+00	2.71039E+04	
HCO3-	HCO3-	1.18472E+00	6.12583E-01	0.5171	5.18230E-02	1.14375E+00	6.97883E+04	
CO2(aq)	CO2(aq)	1.82332E-02	2.32774E-02	1.277	7.97571E-04	1.76026E-02	7.74688E+02	
CO3=	CO3=	1.82316E-02	1.66682E-03	9.1425E-02	7.97499E-04	1.76010E-02	1.05622E+03	-5.18E-08
NaHCO3	Nahcolite	1.24022E-02	1.00000E+00	1.000	5.42505E-04	1.19732E-02	1.00583E+03	1.09E-08
OH-	OH-	8.34088E-07	5.76785E-07	0.6915	3.64853E-08	8.05242E-07	1.36950E-02	1.03E-07
Am(CO3)3=-	Am(CO3)3=-	7.58811E-07	1.95333E-09	2.5742E-03	3.31925E-08	7.32569E-07	3.09897E-01	4.62E-08
H+	H+	3.25455E-08	1.68278E-08	0.5171	1.42363E-09	3.14199E-08	3.16681E-05	-1.06E-07

Figure 6.4.7 Edited Listing of the Output File FMT_AM_NAHC03_QB0204.OUT
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Am(CO3)2-	Am(CO3)2-	3.26281E-09	1.53783E-09	0.4713	1.42724E-10	3.14997E-09	1.14350E-03	9.12E-09
AmCO3+	AmCO3+	3.68368E-11	1.74435E-11	0.4735	1.61134E-12	3.55628E-11	1.07759E-05	-7.63E-08
Am+++	Am+++	1.58846E-12	2.84097E-16	1.7885E-04	6.94835E-14	1.53352E-12	3.72645E-07	-2.31E-07
AmOH++	(after_Cm(III))	1.22787E-16	4.51099E-18	3.6738E-02	5.37103E-18	1.18540E-16	3.08213E-11	-8.11E-08
Am(OH)3(aq)	(le-9m_minimum)	8.63586E-18	8.63586E-18	1.000	3.77757E-19	8.33720E-18	2.45132E-12	1.52E-07
Am(OH)2+	(after_Cm(III))	3.98386E-18	1.88649E-18	0.4735	1.74265E-19	3.84608E-18	1.06542E-12	4.29E-08
Total G/RT=	-5.68168409E+03							

TITRATE file name is WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AM_NAHC03_QB0204.TITRATE;1

Figure 6.4.8 Edited Listing of the Output File FMT_AM_NAHCO3_QB0204.TITRATE
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Benchmark: Solubility of NaAm(CO3)2.6H2O(s) versus NaHCO3
FMT_pH_970407.chemdat
Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5=== by analogy

FMT V2.4

Titrant Volumes per Grid Block, in milliliters

1	0.000000 mL
2	0.121000 mL
3	0.242000 mL
4	0.363000 mL
5	0.484000 mL
6	0.605000 mL
7	0.726000 mL
8	0.847000 mL
9	0.968000 mL
10	1.089000 mL
11	1.210000 mL
12	1.331000 mL
13	1.452000 mL
14	1.573000 mL
15	1.694000 mL
16	1.815000 mL
17	1.936000 mL
18	2.057000 mL
19	2.178000 mL
20	2.299000 mL
21	2.420000 mL
22	2.541000 mL
23	2.662000 mL
24	2.783000 mL
25	2.904000 mL
26	3.025000 mL
27	3.146000 mL
28	3.267000 mL
29	3.388000 mL
30	3.509000 mL
31	3.630000 mL
32	3.751000 mL
33	3.872000 mL
34	3.993000 mL
35	4.114000 mL
36	4.235000 mL
37	4.356000 mL
38	4.477000 mL
39	4.598000 mL
40	4.719000 mL

Titration Results, molal

0)	H2O	Na+	H+
1)	2.17475E+00	7.35404E-02	9.78995E-09
2)	2.18104E+00	1.05620E-01	1.09451E-08
3)	2.18754E+00	1.38567E-01	1.19886E-08
4)	2.19404E+00	1.71320E-01	1.29307E-08
5)	2.20054E+00	2.03879E-01	1.37994E-08
6)	2.20704E+00	2.36246E-01	1.46119E-08
7)	2.21354E+00	2.68424E-01	1.53796E-08
8)	2.22004E+00	3.00412E-01	1.61108E-08
9)	2.22654E+00	3.32214E-01	1.68113E-08
10)	2.23304E+00	3.63831E-01	1.74857E-08
11)	2.23954E+00	3.95264E-01	1.81375E-08
12)	2.24605E+00	4.26515E-01	1.87697E-08
13)	2.25255E+00	4.57586E-01	1.93845E-08
14)	2.25905E+00	4.88478E-01	1.99837E-08
15)	2.26555E+00	5.19192E-01	2.05691E-08
16)	2.27205E+00	5.49731E-01	2.11419E-08
17)	2.27855E+00	5.80095E-01	2.17032E-08

Information Only

Figure 6.4.8 Edited Listing of the Output File FMT_AM_NAHCO3_QB0204.TITRATE
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18)	2.28506E+00	6.10287E-01	2.22541E-08	
19)	2.29156E+00	6.40307E-01	2.27953E-08	
20)	2.29806E+00	6.70157E-01	2.33277E-08	
21)	2.30456E+00	6.99839E-01	2.38519E-08	
22)	2.31106E+00	7.29354E-01	2.43684E-08	
23)	2.31757E+00	7.58703E-01	2.48777E-08	
24)	2.32407E+00	7.87888E-01	2.53803E-08	
25)	2.33057E+00	8.16910E-01	2.58767E-08	
26)	2.33707E+00	8.45771E-01	2.63670E-08	
27)	2.34358E+00	8.74471E-01	2.68518E-08	
28)	2.35008E+00	9.03013E-01	2.73312E-08	
29)	2.35658E+00	9.31397E-01	2.78056E-08	
30)	2.36308E+00	9.59625E-01	2.82751E-08	
31)	2.36959E+00	9.87698E-01	2.87400E-08	
32)	2.37609E+00	1.01562E+00	2.92005E-08	
33)	2.38259E+00	1.04338E+00	2.96568E-08	
34)	2.38909E+00	1.07100E+00	3.01090E-08	
35)	2.39560E+00	1.09846E+00	3.05574E-08	
36)	2.40210E+00	1.12578E+00	3.10019E-08	
37)	2.40860E+00	1.15295E+00	3.14429E-08	
38)	2.41511E+00	1.17997E+00	3.18803E-08	
39)	2.42161E+00	1.20685E+00	3.23144E-08	
40)	2.42810E+00	1.22119E+00	3.25455E-08	
0)	OH-	HCO3-	CO3=	CO2 (aq)
1)	1.66896E-06	7.17417E-02	8.98457E-04	9.00252E-04
2)	1.59766E-06	1.02969E-01	1.32426E-03	1.32599E-03
3)	1.53942E-06	1.35023E-01	1.77150E-03	1.77318E-03
4)	1.49079E-06	1.66871E-01	2.22346E-03	2.22511E-03
5)	1.44865E-06	1.98520E-01	2.67852E-03	2.68013E-03
6)	1.41121E-06	2.29974E-01	3.13559E-03	3.13717E-03
7)	1.37736E-06	2.61234E-01	3.59396E-03	3.59552E-03
8)	1.34633E-06	2.92304E-01	4.05311E-03	4.05465E-03
9)	1.31759E-06	3.23187E-01	4.51267E-03	4.51419E-03
10)	1.29077E-06	3.53884E-01	4.97237E-03	4.97387E-03
11)	1.26555E-06	3.84398E-01	5.43199E-03	5.43348E-03
12)	1.24173E-06	4.14731E-01	5.89136E-03	5.89284E-03
13)	1.21912E-06	4.44883E-01	6.35037E-03	6.35184E-03
14)	1.19758E-06	4.74858E-01	6.80890E-03	6.81036E-03
15)	1.17699E-06	5.04656E-01	7.26688E-03	7.26833E-03
16)	1.15726E-06	5.34280E-01	7.72423E-03	7.72568E-03
17)	1.13832E-06	5.63732E-01	8.18090E-03	8.18235E-03
18)	1.12008E-06	5.93011E-01	8.63685E-03	8.63829E-03
19)	1.10249E-06	6.22121E-01	9.09202E-03	9.09346E-03
20)	1.08551E-06	6.51063E-01	9.54639E-03	9.54783E-03
21)	1.06908E-06	6.79837E-01	9.99993E-03	1.00014E-02
22)	1.05317E-06	7.08447E-01	1.04526E-02	1.04540E-02
23)	1.03775E-06	7.36893E-01	1.09044E-02	1.09058E-02
24)	1.02279E-06	7.65176E-01	1.13553E-02	1.13567E-02
25)	1.00825E-06	7.93298E-01	1.18052E-02	1.18067E-02
26)	9.94119E-07	8.21260E-01	1.22542E-02	1.22557E-02
27)	9.80372E-07	8.49065E-01	1.27023E-02	1.27037E-02
28)	9.66988E-07	8.76712E-01	1.31494E-02	1.31508E-02
29)	9.53950E-07	9.04204E-01	1.35954E-02	1.35969E-02
30)	9.41241E-07	9.31541E-01	1.40405E-02	1.40420E-02
31)	9.28846E-07	9.58726E-01	1.44845E-02	1.44860E-02
32)	9.16751E-07	9.85759E-01	1.49276E-02	1.49291E-02
33)	9.04943E-07	1.01264E+00	1.53695E-02	1.53711E-02
34)	8.93411E-07	1.03938E+00	1.58104E-02	1.58120E-02
35)	8.82143E-07	1.06596E+00	1.62503E-02	1.62518E-02
36)	8.71129E-07	1.09240E+00	1.66891E-02	1.66906E-02
37)	8.60360E-07	1.11869E+00	1.71267E-02	1.71283E-02
38)	8.49825E-07	1.14484E+00	1.75633E-02	1.75649E-02
39)	8.39518E-07	1.17085E+00	1.79988E-02	1.80004E-02
40)	8.34088E-07	1.18472E+00	1.82316E-02	1.82332E-02

0) Am+++

Information Only

Figure 6.4.8 Edited Listing of the Output File FMT_AM_NAHCO3_QB0204.TITRATE
(Page 3 of 5)

- 1) 1.07521E-12
- 2) 7.66585E-13
- 3) 6.33388E-13
- 4) 5.67790E-13
- 5) 5.33478E-13
- 6) 5.16283E-13
- 7) 5.09607E-13
- 8) 5.09985E-13
- 9) 5.15436E-13
- 10) 5.24753E-13
- 11) 5.37162E-13
- 12) 5.52149E-13
- 13) 5.69362E-13
- 14) 5.88554E-13
- 15) 6.09549E-13
- 16) 6.32222E-13
- 17) 6.56481E-13
- 18) 6.82261E-13
- 19) 7.09514E-13
- 20) 7.38209E-13
- 21) 7.68323E-13
- 22) 7.99844E-13
- 23) 8.32765E-13
- 24) 8.67084E-13
- 25) 9.02805E-13
- 26) 9.39934E-13
- 27) 9.78481E-13
- 28) 1.01846E-12
- 29) 1.05988E-12
- 30) 1.10275E-12
- 31) 1.14711E-12
- 32) 1.19295E-12
- 33) 1.24031E-12
- 34) 1.28919E-12
- 35) 1.33963E-12
- 36) 1.39164E-12
- 37) 1.44525E-12
- 38) 1.50047E-12
- 39) 1.55732E-12
- 40) 1.58846E-12

	AmCO3+	Am(CO3)2-	Am(CO3)3--	AmOH++	Am(OH)2+	Am(OH)3(aq)
1)	1.03314E-09	1.83893E-08	3.73302E-08	7.24537E-15	2.94848E-15	2.39019E-14
2)	6.11347E-10	1.39822E-08	4.80079E-08	3.58638E-15	1.17576E-15	8.49698E-15
3)	4.18762E-10	1.14745E-08	5.87747E-08	2.18166E-15	5.97683E-16	3.92992E-15
4)	3.14538E-10	9.88188E-09	6.94575E-08	1.50771E-15	3.55047E-16	2.15712E-15
5)	2.50354E-10	8.77289E-09	8.01727E-08	1.12796E-15	2.32859E-16	1.32125E-15
6)	2.07335E-10	7.95220E-09	9.10035E-08	8.90423E-16	1.63523E-16	8.73325E-16
7)	1.76725E-10	7.31802E-09	1.02014E-07	7.30571E-16	1.20713E-16	6.10481E-16
8)	1.53954E-10	6.81187E-09	1.13258E-07	6.17024E-16	9.25657E-17	4.45419E-16
9)	1.36424E-10	6.39766E-09	1.24779E-07	5.32952E-16	7.31368E-17	3.36164E-16
10)	1.22555E-10	6.05184E-09	1.36618E-07	4.68628E-16	5.91964E-17	2.60747E-16
11)	1.11337E-10	5.75839E-09	1.48809E-07	4.18090E-16	4.88733E-17	2.06871E-16
12)	1.02094E-10	5.50597E-09	1.61385E-07	3.77502E-16	4.10258E-17	1.67269E-16
13)	9.43600E-11	5.28635E-09	1.74377E-07	3.44302E-16	3.49270E-17	1.37448E-16
14)	8.78026E-11	5.09341E-09	1.87813E-07	3.16718E-16	3.00967E-17	1.14525E-16
15)	8.21790E-11	4.92245E-09	2.01721E-07	2.93489E-16	2.62080E-17	9.65853E-17
16)	7.73083E-11	4.76987E-09	2.16127E-07	2.73701E-16	2.30326E-17	8.23253E-17
17)	7.30527E-11	4.63279E-09	2.31056E-07	2.56669E-16	2.04067E-17	7.08328E-17
18)	6.93056E-11	4.50894E-09	2.46533E-07	2.41878E-16	1.82111E-17	6.14567E-17
19)	6.59836E-11	4.39646E-09	2.62584E-07	2.28931E-16	1.63569E-17	5.37233E-17
20)	6.30202E-11	4.29385E-09	2.79231E-07	2.17515E-16	1.47769E-17	4.72817E-17
21)	6.03620E-11	4.19985E-09	2.96499E-07	2.07385E-16	1.34197E-17	4.18682E-17
22)	5.79656E-11	4.11341E-09	3.14412E-07	1.98345E-16	1.22454E-17	3.72820E-17
23)	5.57952E-11	4.03366E-09	3.32993E-07	1.90233E-16	1.12225E-17	3.33678E-17
24)	5.38213E-11	3.95984E-09	3.52267E-07	1.82921E-16	1.03260E-17	3.00047E-17
25)	5.20192E-11	3.89133E-09	3.72257E-07	1.76300E-16	9.53600E-18	2.70970E-17
26)	5.03682E-11	3.82757E-09	3.92987E-07	1.70281E-16	8.83614E-18	2.45687E-17

Figure 6.4.8 Edited Listing of the Output File FMT_AM_NAHC03_QB0204.TITRATE
 (Page 4 of 5)

27)	4.88507E-11	3.76809E-09	4.14481E-07	1.64789E-16	8.21320E-18	2.23587E-17
28)	4.74517E-11	3.71248E-09	4.36762E-07	1.59761E-16	7.65628E-18	2.04173E-17
29)	4.61583E-11	3.66039E-09	4.59855E-07	1.55143E-16	7.15632E-18	1.87040E-17
30)	4.49595E-11	3.61148E-09	4.83785E-07	1.50890E-16	6.70578E-18	1.71858E-17
31)	4.38457E-11	3.56550E-09	5.08576E-07	1.46961E-16	6.29833E-18	1.58349E-17
32)	4.28085E-11	3.52219E-09	5.34253E-07	1.43323E-16	5.92860E-18	1.46284E-17
33)	4.18405E-11	3.48133E-09	5.60840E-07	1.39946E-16	5.59205E-18	1.35471E-17
34)	4.09355E-11	3.44273E-09	5.88363E-07	1.36805E-16	5.28480E-18	1.25749E-17
35)	4.00877E-11	3.40621E-09	6.16847E-07	1.33878E-16	5.00352E-18	1.16980E-17
36)	3.92922E-11	3.37162E-09	6.46318E-07	1.31143E-16	4.74533E-18	1.09047E-17
37)	3.85444E-11	3.33881E-09	6.76801E-07	1.28585E-16	4.50776E-18	1.01851E-17
38)	3.78404E-11	3.30767E-09	7.08323E-07	1.26187E-16	4.28865E-18	9.53068E-18
39)	3.71768E-11	3.27806E-09	7.40911E-07	1.23936E-16	4.08610E-18	8.93396E-18
40)	3.68368E-11	3.26281E-09	7.58811E-07	1.22787E-16	3.98386E-18	8.63586E-18

0)		NaAm(CO3) 2.6H				
1)	1.07268E-03	9.92624E+01				
2)	0.00000E+00	9.89773E+01				
3)	0.00000E+00	9.86832E+01				
4)	0.00000E+00	9.83908E+01				
5)	0.00000E+00	9.81002E+01				
6)	0.00000E+00	9.78112E+01				
7)	0.00000E+00	9.75240E+01				
8)	0.00000E+00	9.72384E+01				
9)	0.00000E+00	9.69545E+01				
10)	0.00000E+00	9.66722E+01				
11)	0.00000E+00	9.63916E+01				
12)	0.00000E+00	9.61126E+01				
13)	0.00000E+00	9.58351E+01				
14)	0.00000E+00	9.55593E+01				
15)	0.00000E+00	9.52851E+01				
16)	0.00000E+00	9.50124E+01				
17)	0.00000E+00	9.47413E+01				
18)	0.00000E+00	9.44717E+01				
19)	0.00000E+00	9.42037E+01				
20)	0.00000E+00	9.39372E+01				
21)	0.00000E+00	9.36721E+01				
22)	0.00000E+00	9.34086E+01				
23)	0.00000E+00	9.31465E+01				
24)	0.00000E+00	9.28859E+01				
25)	0.00000E+00	9.26267E+01				
26)	0.00000E+00	9.23690E+01				
27)	0.00000E+00	9.21127E+01				
28)	0.00000E+00	9.18579E+01				
29)	0.00000E+00	9.16044E+01				
30)	0.00000E+00	9.13523E+01				
31)	0.00000E+00	9.11016E+01				
32)	0.00000E+00	9.08523E+01				
33)	0.00000E+00	9.06043E+01				
34)	0.00000E+00	9.03577E+01				
35)	0.00000E+00	9.01124E+01				
36)	0.00000E+00	8.98685E+01				
37)	0.00000E+00	8.96259E+01				
38)	0.00000E+00	8.93845E+01				
39)	0.00000E+00	8.91445E+01				
40)	0.00000E+00	8.89060E+01				

0)	IonicStrength	Titrvol,ml	pH	pmH
1)	7.44390E-02	0.000000000E+00	8.122	8.009
2)	1.06944E-01	0.121000000	8.091	7.961
3)	1.40339E-01	0.242000000	8.066	7.921
4)	1.73544E-01	0.363000000	8.045	7.888
5)	2.06558E-01	0.484000000	8.027	7.860
6)	2.39382E-01	0.605000000	8.011	7.835
7)	2.72018E-01	0.726000000	7.997	7.813
8)	3.04466E-01	0.847000000	7.984	7.793

Figure 6.4.8 Edited Listing of the Output File FMT_AM_NAHCO3_QB0204.TITRATE
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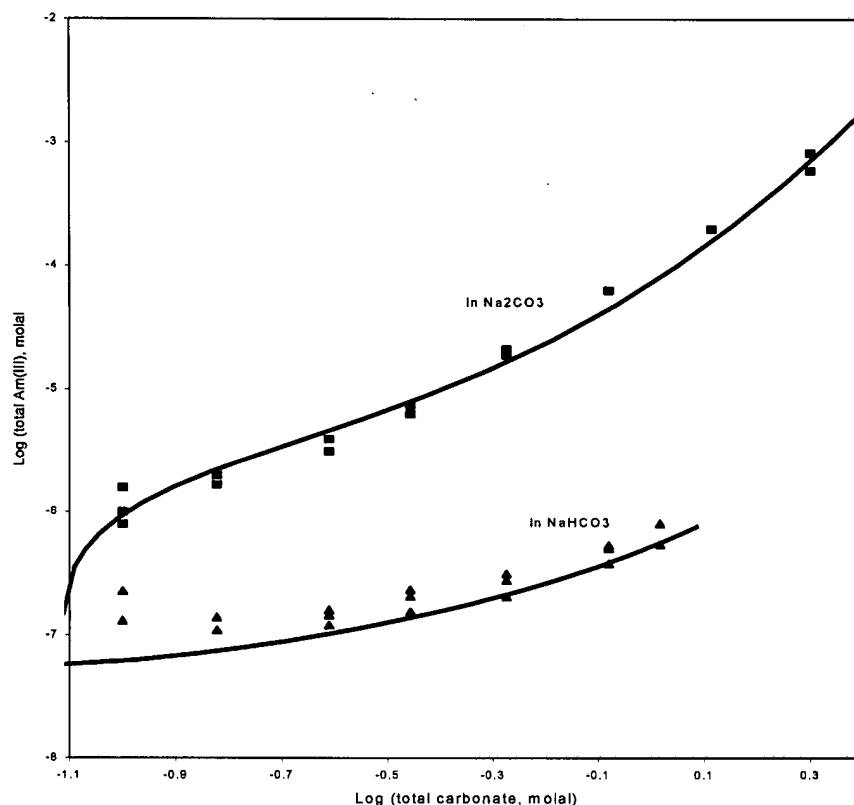
9)	3.36727E-01	0.968000000	7.972	7.774
10)	3.68804E-01	1.089000000	7.961	7.757
11)	4.00696E-01	1.210000000	7.951	7.741
12)	4.32407E-01	1.331000000	7.941	7.727
13)	4.63937E-01	1.452000000	7.932	7.713
14)	4.95287E-01	1.573000000	7.923	7.699
15)	5.26460E-01	1.694000000	7.915	7.687
16)	5.57456E-01	1.815000000	7.907	7.675
17)	5.88277E-01	1.936000000	7.899	7.663
18)	6.18924E-01	2.057000000	7.892	7.653
19)	6.49400E-01	2.178000000	7.885	7.642
20)	6.79705E-01	2.299000000	7.878	7.632
21)	7.09840E-01	2.420000000	7.871	7.622
22)	7.39808E-01	2.541000000	7.865	7.613
23)	7.69609E-01	2.662000000	7.859	7.604
24)	7.99245E-01	2.783000000	7.853	7.596
25)	8.28717E-01	2.904000000	7.847	7.587
26)	8.58026E-01	3.025000000	7.841	7.579
27)	8.87175E-01	3.146000000	7.835	7.571
28)	9.16164E-01	3.267000000	7.830	7.563
29)	9.44994E-01	3.388000000	7.824	7.556
30)	9.73667E-01	3.509000000	7.819	7.549
31)	1.00218E+00	3.630000000	7.814	7.542
32)	1.03055E+00	3.751000000	7.809	7.535
33)	1.05875E+00	3.872000000	7.804	7.528
34)	1.08681E+00	3.993000000	7.799	7.521
35)	1.11472E+00	4.114000000	7.795	7.515
36)	1.14247E+00	4.235000000	7.790	7.509
37)	1.17008E+00	4.356000000	7.785	7.502
38)	1.19754E+00	4.477000000	7.781	7.496
39)	1.22485E+00	4.598000000	7.776	7.491
40)	1.23942E+00	4.719000000	7.774	7.488

6.4.4 Evaluation

The calculated $\text{NaAm}(\text{CO}_3)_2 \cdot 6\text{H}_2\text{O}$ solubility was to be graphically compared with the experimental data from Rao et al. (1996). The model prediction was to follow the general trend of the experimental data and the deviation of the model prediction from the experimental data was expected to be less than half a logarithmic unit.

Figures 6.4.5 and 6.4.7 show the nonzero concentrations calculated by FMT. Figures 6.4.6 and 6.4.8 show the nonzero titration results calculated by FMT. Figure 6.4.9 is a graphical comparison of total Am(III) concentrations calculated by FMT with the experimental data from Rao et al. (1996). It can be seen that the model prediction follows the general trend of the experimental data and the deviation of the model prediction from the experimental measurements is less than half a logarithmic unit. Therefore, the acceptance criteria is considered to have been met.

Figure 6.4.9 Comparison of Total Am(III) Concentrations Calculated by FMT with Experimental Data



6.5 Test Case #5: Solubility of AmPO₄ in Na₂SO₄ Solutions

6.5.1 Test Objectives

Using the "titration" mode of logarithmic increments, FMT calculates the solubility of AmPO₄ in both 10^{-2.06} m and 10^{-1.12} m Na₂SO₄ solutions as a function of pcH. The solution pcH change was to be made by adding HCl. It tests functional requirements R.2, R.4, and R.7.

6.5.2 Test Procedures

This test case was run using the script FMT_TEST_QB0204.COM. This command file is shown in **Figure 6.0.2**.

6.5.3 Input/Output Files

The following is a list of all files associated with Test Case #5:

Command file:

FMT_TEST_QB0204.COM

Input files:

FMT_AMPO4_SO4_BM1.IN (See **Figure 6.5.1**)

FMT_AMPO4_SO4_BM1.INGUESS (See **Figure 6.5.2**)

FMT_AMPO4_SO4_BM2.IN (See **Figure 6.5.3**)

FMT_AMPO4_SO4_BM2.INGUESS (See **Figure 6.5.4**)

Output files:

FMT_AMPO4_SO4_BM1_QB0204.OUT (See **Figure 6.5.5**)

FMT_AMPO4_SO4_BM1_QB0204.TITRATE (See **Figure 6.5.6**)

FMT_AMPO4_SO4_BM2_QB0204.OUT (See **Figure 6.5.7**)

FMT_AMPO4_SO4_BM2_QB0204.TITRATE (See **Figure 6.5.8**)

Figure 6.5.1 Listing of the Input File FMT_AMPO4_SO4_BM1.IN
(Page 1 of 2)

```
'Fig 5, Rai et al 1994, AmPO4(c) Solubility in 10^-3.06 M SO4= Media'  
'CHEMFILE'  
'TITRATE' 'EXPLICIT'  
'DISABLE_SPECIES' 0  
'nSET_FC02' 0.0  
'nSET_PH' 0.0  
  
'nMOLES' 'nEXACT'  
1.21017364E+02 Hydrogen  
5.55086820E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
10.d0 0000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Pu(III)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL  
  
'nMOLES' 'nEXACT'  
1.11017996E+02 Hydrogen AmPO4(c) w/10^3.5M NaH2PO4 and 10^-3.06M Na2SO4  
9.55134308E+01 Oxygen  
2.05820000E-03 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
8.71000000E-04 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
1.00000000E+01 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
1.00003162E+01 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
-3.43912739E-19 Charge:EL  
  
15 2.25d3 0.0025d0 1.800001d5 'NDXVARIABLE'  
'nDIFFUS',  
'CONVEC',
```

Figure 6.5.1 Listing of the Input File FMT_AMPO4_SO4_BM1.IN
(Page 2 of 2)

```
'nSSDIFF',  
'nRESTART',  
'nPUSHPULL', 'nMULTINJ',  
  
20 1 20 'nLOTS' 10  
'nTGRAD' 'LINEAR'  
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'  
3  
0.1d0 0.2d0 0.3d0  
1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'  
'nMOLES' 'nEXACT' Plain old pure H2O  
1.11017364E+02 Hydrogen  
5.55086820E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Pu(III)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL  
  
1.d-12 1.d-20 (fracture, matrix permeabilities)  
'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)  
'VAR_AQ_RHO' 1074.9d0  
'nNO X DIFF',  
'UNIFORM', 0  
  
'TITRATE', 'LOG10', 0.01d0, 1.7d0, 'nINJSOLIDS'
```

Figure 6.5.2 Listing of the Input File FMT_AMPO4_SO4_BM1.INGUESS
(Page 1 of 2)

```
5.550868189957750E+01 H2O WATER 5.550868155779565E+01
3.162d-4 0.000000000000000E+00 Na+ Na+ 0.000000000000000E+00
0.000000000000000E+00 K+ K+ 0.000000000000000E+00
0.000000000000000E+00 Ca++ Ca++ 0.000000000000000E+00
0.000000000000000E+00 Mg++ Mg++ 0.000000000000000E+00
0.000000000000000E+00 MgOH+ MgOH+ 0.000000000000000E+00
1.004224980959840E-07 H+ H+ 1.004224974776557E-07
0.000000000000000E+00 Cl- Cl- 0.000000000000000E+00
1.d-20 0.000000000000000E+00 SO4= SO4= 0.000000000000000E+00
0.000000000000000E+00 HSO4- HSO4- 0.000000000000000E+00
1.004224980959840E-07 OH- OH- 1.004224974776557E-07
0.000000000000000E+00 HCO3- HCO3- 0.000000000000000E+00
0.000000000000000E+00 CO3= CO3= 0.000000000000000E+00
0.000000000000000E+00 CO2 (aq) CO2 (aq) 0.000000000000000E+00
0.000000000000000E+00 CaCO3 (aq) CaCO3 (aq) 0.000000000000000E+00
0.000000000000000E+00 MgCO3 (aq) MgCO3 (aq) 0.000000000000000E+00
0.000000000000000E+00 B(OH)3 (aq) B(OH)3 (aq) 0.000000000000000E+00
0.000000000000000E+00 B(OH)4- B(OH)4- 0.000000000000000E+00
0.000000000000000E+00 B3O3(OH)4- B3O3(OH)4- 0.000000000000000E+00
0.000000000000000E+00 B4O5(OH)4= B4O5(OH)4= 0.000000000000000E+00
0.000000000000000E+00 CaB(OH)4+ CaB(OH)4+ 0.000000000000000E+00
0.000000000000000E+00 MgB(OH)4+ MgB(OH)4+ 0.000000000000000E+00
0.000000000000000E+00 Br- Br- 0.000000000000000E+00
0.000000000000000E+00 ClO4- perchlorate ClO4- 0.000000000000000E+00
0.000000000000000E+00 NaOH(aq).....to.titrate.base.only NaOH(aq).....to.titrate.base.only 0.000000000000000E+00
0.000000000000000E+00 HCl(aq).....to.titrate.acid.only HCl(aq).....to.titrate.acid.only 0.000000000000000E+00
0.000000000000000E+00 HClO4(aq).....to.titrate.acid.only HClO4(aq).....to.titrate.acid.only 0.000000000000000E+00
0.000000000000000E+00 PosIon..... POSITIVE.ION PosIon..... POSITIVE.ION 0.000000000000000E+00
0.000000000000000E+00 NegIon..... NEGATIVE.ION NegIon..... NEGATIVE.ION 0.000000000000000E+00
0.000000000000000E+00 PosIon(OH)(aq).....to.titrate.base PosIon(OH)(aq).....to.titrate.base 0.000000000000000E+00
0.000000000000000E+00 HNegIon(aq).....to.titrate.acid HNegIon(aq).....to.titrate.acid 0.000000000000000E+00
0.000000000000000E+00 Tracer(aq).....conservative.tracer Tracer(aq).....conservative.tracer 0.000000000000000E+00
0.000000000000000E+00 H3PO4(aq) H3PO4(aq) 0.000000000000000E+00
3.162d-4 0.000000000000000E+00 H2PO4- H2PO4- 0.000000000000000E+00
0.000000000000000E+00 HPO4= HPO4= 0.000000000000000E+00
0.000000000000000E+00 PO4=- PO4=- 0.000000000000000E+00
0.000000000000000E+00 NpO2+ NpO2+ 0.000000000000000E+00
0.000000000000000E+00 NpO2OH(aq) NpO2OH(aq) 0.000000000000000E+00
0.000000000000000E+00 NpO2(OH)2- NpO2(OH)2- 0.000000000000000E+00
0.000000000000000E+00 NpO2CO3- NpO2CO3- 0.000000000000000E+00
0.000000000000000E+00 NpO2(CO3)2=- NpO2(CO3)2=- 0.000000000000000E+00
0.000000000000000E+00 NpO2(CO3)3=- NpO2(CO3)3=- 0.000000000000000E+00
0.000000000000000E+00 Am+++ Am+++ 0.000000000000000E+00
0.000000000000000E+00 AmCO3+ AmCO3+ 0.000000000000000E+00
0.000000000000000E+00 Am(CO3)2- Am(CO3)2- 0.000000000000000E+00
0.000000000000000E+00 Am(CO3)3=- Am(CO3)3=- 0.000000000000000E+00
0.000000000000000E+00 Am(OH)2+ Am(OH)2+ 0.000000000000000E+00
0.000000000000000E+00 Am(OH)3(aq) Am(OH)3(aq) 0.000000000000000E+00
0.000000000000000E+00 Th++++ Th++++ 0.000000000000000E+00
0.000000000000000E+00 UO2++ U(VI)O2++ 0.000000000000000E+00
0.000000000000000E+00 NpO2OH(aged) NpO2OH(aged) 0.000000000000000E+00
0.000000000000000E+00 NpO2OH(amor) NpO2OH(amor) 0.000000000000000E+00
0.000000000000000E+00 NaNpO2CO3(s) NaNpO2CO3(s) 0.000000000000000E+00
0.000000000000000E+00 Na3NpO2(CO3)2(s)_DISABLED DISABLED 0.000000000000000E+00
0.000000000000000E+00 AmOHC(O3)(c) AmOHC(O3)(c) 0.000000000000000E+00
0.000000000000000E+00 Am(OH)3(s) Am(OH)3(s) 0.000000000000000E+00
0.000000000000000E+00 NaAm(CO3)2.6H2O(c) NaAm(CO3)2.6H2O(c) 0.000000000000000E+00
10.d0 0.000000000000000E+00 AmPO4(c) AmPO4(c) 0.000000000000000E+00
0.000000000000000E+00 CaSO4 Anhydrite 0.000000000000000E+00
0.000000000000000E+00 NaK3(SO4)2 Aphanthalite/Glaserite 0.000000000000000E+00
0.000000000000000E+00 CaCl2.6H2O Antarcticite 0.000000000000000E+00
0.000000000000000E+00 CaCO3 Aragonite 0.000000000000000E+00
0.000000000000000E+00 K2SO4 Arcanite 0.000000000000000E+00
0.000000000000000E+00 MgCl2.6H2O Bischofite 0.000000000000000E+00
0.000000000000000E+00 Na2Mg(SO4)2.4H2O Bloedite 0.000000000000000E+00
0.000000000000000E+00 Mg(OH)2 Brucite 0.000000000000000E+00
0.000000000000000E+00 Na6CO3(SO4)2 Burkeite 0.000000000000000E+00
```

Figure 6.5.2 Listing of the Input File FMT_AMPO4_SO4_BM1.INGUESS
(Page 2 of 2)

0.000000000000000E+00	CaCO3	Calcite	0.000000000000000E+00
0.000000000000000E+00	CaCl2.4H2O	CaCl2_Tetrahydrate	0.000000000000000E+00
0.000000000000000E+00	Ca4Cl2(OH)6.13H2O	CaOxychloride A	0.000000000000000E+00
0.000000000000000E+00	Ca2Cl2(OH)2.2H2O	CaOxychloride B	0.000000000000000E+00
0.000000000000000E+00	KMgCl3.6H2O	Carnallite	0.000000000000000E+00
0.000000000000000E+00	MgSO4.7H2O	Epsomite	0.000000000000000E+00
0.000000000000000E+00	CaNa2(CO3)2.5H2O	Gaylussite	0.000000000000000E+00
0.000000000000000E+00	Na2Ca(SO4)2	Glauberite	0.000000000000000E+00
0.000000000000000E+00	CaSO4.2H2O	Gypsum	0.000000000000000E+00
0.000000000000000E+00	NaCl	Halite	0.000000000000000E+00
0.000000000000000E+00	MgSO4.6H2O	Hexahydrate	0.000000000000000E+00
0.000000000000000E+00	KMgClSO4.3H2O	Kainite	0.000000000000000E+00
0.000000000000000E+00	KHCO3	Kalicinite	0.000000000000000E+00
0.000000000000000E+00	MgSO4.H2O	Kieserite	0.000000000000000E+00
0.000000000000000E+00	K2Mg(SO4)2.4H2O	Leonite	0.000000000000000E+00
0.000000000000000E+00	Na4Ca(SO4)3.2H2O	Labile_Salt	0.000000000000000E+00
0.000000000000000E+00	MgCO3	Magnesite	0.000000000000000E+00
0.000000000000000E+00	Mg2Cl(OH)3.4H2O	MgOxychloride	0.000000000000000E+00
0.000000000000000E+00	KHSO4	Mercallite	0.000000000000000E+00
0.000000000000000E+00	Na2SO4.10H2O	Mirabilite	0.000000000000000E+00
0.000000000000000E+00	K8H6(SO4)7	Misenite	0.000000000000000E+00
0.000000000000000E+00	NaHCO3	Nahcolite	0.000000000000000E+00
0.000000000000000E+00	Na2CO3.10H2O	Natron	0.000000000000000E+00
0.000000000000000E+00	MgCO3.3H2O	Nesquehonite	0.000000000000000E+00
0.000000000000000E+00	K2Mg(SO4)2.6H2O	Picromerite/Schoen	0.000000000000000E+00
0.000000000000000E+00	Na2Ca(CO3)2.2H2O	Pirssonite	0.000000000000000E+00
0.000000000000000E+00	K2MgCa2(SO4)4.2H2O	Polyhalite	0.000000000000000E+00
0.000000000000000E+00	Ca(OH)2	Portlandite	0.000000000000000E+00
0.000000000000000E+00	K2CO3.3/2H2O	Potassium Carbonate	0.000000000000000E+00
0.000000000000000E+00	K8H4(CO3)6.3H2O	K-Sequicarbonate	0.000000000000000E+00
0.000000000000000E+00	KNaCO3.6H2O	K-Na-Carbonate	0.000000000000000E+00
0.000000000000000E+00	K2NaH(CO3)2.2H2O	Potassium Trona	0.000000000000000E+00
0.000000000000000E+00	K3H(SO4)2	Sesquipotassium Sulfate	0.000000000000000E+00
0.000000000000000E+00	Na3H(SO4)2	Sesquisodium Sulfate	0.000000000000000E+00
0.000000000000000E+00	Na2CO3.7H2O	Na2CO3-Heptahydrate	0.000000000000000E+00
0.000000000000000E+00	KCl	Sylvite	0.000000000000000E+00
0.000000000000000E+00	K2Ca(SO4)2.H2O	Syngenite	0.000000000000000E+00
0.000000000000000E+00	Mg2CaCl6.12H2O	Tachyhydrite	0.000000000000000E+00
7.586d-2	0.000000000000000E+00	Na2SO4	Thenardite 0.000000000000000E+00
0.000000000000000E+00	Na2CO3.H2O	Thermonatrite	0.000000000000000E+00
0.000000000000000E+00	Na3H(CO3)2.2H2O	Trona	0.000000000000000E+00
0.000000000000000E+00	Na2B4O7.10H2O	Borax	0.000000000000000E+00
0.000000000000000E+00	B(OH)3	Borix Acid_Solid	0.000000000000000E+00
0.000000000000000E+00	KB5O8.4H2O	K-Pentaborate_(30_C)	0.000000000000000E+00
0.000000000000000E+00	K2B4O7.4H2O	K-Tetraborate_(30_C)	0.000000000000000E+00
0.000000000000000E+00	NaBO2.4H2O	Sodium Metaborate	0.000000000000000E+00
0.000000000000000E+00	NaB5O8.5H2O	Sodium Pentaborate	0.000000000000000E+00
0.000000000000000E+00	NaBO2.NaCl.2H2O	Teepelite_(20_C)	0.000000000000000E+00

Figure 6.5.3 Listing of the Input File FMT_AMPO4_SO4_BM2.IN
(Page 1 of 2)

```
'Fig 5, Rai et al 1994, AmPO4(c) Solubility in 10^-1.12 M SO4= Media'  
'CHEMFILE'  
'TITRATE' 'EXPLICIT'  
'DISABLE_SPECIES' 0.0  
'nSET_FC02' 0.0  
'nSET_PH' 0.0  
  
'nMOLES' 'nEXACT'  
1.21017364E+02 Hydrogen  
5.55086820E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
10.d0 0000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Pu(III)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL  
  
'nMOLES' 'nEXACT'  
1.11017996E+02 Hydrogen AmPO4(c) w/10^3.5M NaH2PO4 and 10^-1.12M Na2SO4  
9.58133868E+01 Oxygen  
1.52036200E-01 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
7.58600000E-02 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
1.00000000E+01 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
1.00003162E+01 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
-9.82070136E-18 Charge:EL  
  
15 2.25d3 0.0025d0 1.800001d5 'ndxVARIABLE'  
'nDIFFUS',  
'CONVEC',
```

Figure 6.5.3 Listing of the Input File FMT_AMPO4_SO4_BM2.IN
(Page 2 of 2)

```
'nSSDIFF',  
'nRESTART',  
'nPUSHPULL', 'nMULTINJ',  
  
20 1 20 'nLOTS' 10  
'nTGRAD' 'LINEAR'  
'FRAC FLO' 'nTWO PHASE' 'nMASS TR'  
3  
0.1d0 0.2d0 0.3d0  
1.d-7 0.d0 0.18291d0 0.2d0 0.d0 'RHSFDIF' 'LHSFDIF'  
'nMOLES' 'nEXACT' Plain old pure H2O  
1.11017364E+02 Hydrogen  
5.55086820E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Pu(III)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:El  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL  
  
1.d-12 1.d-20 (fracture, matrix permeabilities)  
'VPOROS' 'FRFLASH' (NOFLASH or FRFLASH, default is all flash)  
'VAR AQ_RHO' 1074.9d0  
'nNO_X DIFF',  
'UNIFORM',0  
  
'TITRATE', 'LOG10', 0.01d0, 2.0d0, 'nINJSOLIDS'
```


Figure 6.5.4 Listing of the Input File FMT_AMPO4_SO4_BM2.INGUESS
(Page 1 of 2)

```
5.550868189957750E+01 H2O WATER 5.550868155779565E+01
3.162d-4 0.000000000000000E+00 Na+ Na+ 0.000000000000000E+00
0.000000000000000E+00 K+ K+ 0.000000000000000E+00
0.000000000000000E+00 Ca++ Ca++ 0.000000000000000E+00
0.000000000000000E+00 Mg++ Mg++ 0.000000000000000E+00
0.000000000000000E+00 MgOH+ MgOH+ 0.000000000000000E+00
1.004224980959840E-07 H+ H+ 1.004224974776557E-07
0.000000000000000E+00 Cl- Cl- 0.000000000000000E+00
1.d-20 0.000000000000000E+00 SO4= SO4= 0.000000000000000E+00
0.000000000000000E+00 HSO4- HSO4- 0.000000000000000E+00
1.004224980959840E-07 OH- OH- 1.004224974776557E-07
0.000000000000000E+00 HCO3- HCO3- 0.000000000000000E+00
0.000000000000000E+00 CO3= CO3= 0.000000000000000E+00
0.000000000000000E+00 CO2 (aq) CO2 (aq) 0.000000000000000E+00
0.000000000000000E+00 CaCO3 (aq) CaCO3 (aq) 0.000000000000000E+00
0.000000000000000E+00 MgCO3 (aq) MgCO3 (aq) 0.000000000000000E+00
0.000000000000000E+00 B (OH) 3 (aq) B (OH) 3 (aq) 0.000000000000000E+00
0.000000000000000E+00 B (OH) 4- B (OH) 4- 0.000000000000000E+00
0.000000000000000E+00 B3O3 (OH) 4- B3O3 (OH) 4- 0.000000000000000E+00
0.000000000000000E+00 B4O5 (OH) 4= B4O5 (OH) 4= 0.000000000000000E+00
0.000000000000000E+00 CaB (OH) 4+ CaB (OH) 4+ 0.000000000000000E+00
0.000000000000000E+00 MgB (OH) 4+ MgB (OH) 4+ 0.000000000000000E+00
0.000000000000000E+00 Br- Br- 0.000000000000000E+00
0.000000000000000E+00 ClO4- perchlorate ClO4- 0.000000000000000E+00
0.000000000000000E+00 NaOH (aq).....to.titrate.base.only 0.000000000000000E+00
0.000000000000000E+00 HCl (aq).....to.titrate.acid.only 0.000000000000000E+00
0.000000000000000E+00 HClO4 (aq).....to.titrate.acid.only 0.000000000000000E+00
0.000000000000000E+00 PosIon..... POSITIVE. ION 0.000000000000000E+00
0.000000000000000E+00 NegIon..... NEGATIVE. ION 0.000000000000000E+00
0.000000000000000E+00 PosIon(OH) (aq).....to.titrate.base 0.000000000000000E+00
0.000000000000000E+00 HNegIon (aq).....to.titrate.acid 0.000000000000000E+00
0.000000000000000E+00 Tracer (aq).....conservative.tracer 0.000000000000000E+00
0.000000000000000E+00 H3PO4 (aq) H3PO4 (aq) 0.000000000000000E+00
3.162d-4 0.000000000000000E+00 H2PO4- H2PO4- 0.000000000000000E+00
0.000000000000000E+00 HPO4= HPO4= 0.000000000000000E+00
0.000000000000000E+00 PO4=- PO4=- 0.000000000000000E+00
0.000000000000000E+00 NpO2+ NpO2+ 0.000000000000000E+00
0.000000000000000E+00 NpO2OH (aq) NpO2OH (aq) 0.000000000000000E+00
0.000000000000000E+00 NpO2 (OH) 2- NpO2 (OH) 2- 0.000000000000000E+00
0.000000000000000E+00 NpO2CO3- NpO2CO3- 0.000000000000000E+00
0.000000000000000E+00 NpO2 (CO3) 2=- NpO2 (CO3) 2=- 0.000000000000000E+00
0.000000000000000E+00 NpO2 (CO3) 3=- NpO2 (CO3) 3=- 0.000000000000000E+00
0.000000000000000E+00 Am+++ Am+++ 0.000000000000000E+00
0.000000000000000E+00 AmCO3+ AmCO3+ 0.000000000000000E+00
0.000000000000000E+00 Am (CO3) 2- Am (CO3) 2- 0.000000000000000E+00
0.000000000000000E+00 Am (CO3) 3=- Am (CO3) 3=- 0.000000000000000E+00
0.000000000000000E+00 Am (OH) 2+ Am (OH) 2+ 0.000000000000000E+00
0.000000000000000E+00 Am (OH) 3 (aq) Am (OH) 3 (aq) 0.000000000000000E+00
0.000000000000000E+00 Th++++ Th++++ 0.000000000000000E+00
0.000000000000000E+00 UO2++ U (VI) O2++ 0.000000000000000E+00
0.000000000000000E+00 NpO2OH (aged) NpO2OH (aged) 0.000000000000000E+00
0.000000000000000E+00 NpO2OH (amor) NpO2OH (amor) 0.000000000000000E+00
0.000000000000000E+00 NaNpO2CO3 (s) NaNpO2CO3 (s) 0.000000000000000E+00
0.000000000000000E+00 Na3NpO2 (CO3) 2 (s) DISABLED DISABLED 0.000000000000000E+00
0.000000000000000E+00 AmOHCO3 (c) AmOHCO3 (c) 0.000000000000000E+00
0.000000000000000E+00 Am (OH) 3 (s) Am (OH) 3 (s) 0.000000000000000E+00
0.000000000000000E+00 NaAm (CO3) 2.6H2O (c) 0.000000000000000E+00
10.d0 0.000000000000000E+00 AmPO4 (c) AmPO4 (c) 0.000000000000000E+00
0.000000000000000E+00 CaSO4 Anhydrite 0.000000000000000E+00
0.000000000000000E+00 NaK3 (SO4) 2 Aphanthalite/Glaserite 0.000000000000000E+00
0.000000000000000E+00 CaCl2.6H2O Antarcticite 0.000000000000000E+00
0.000000000000000E+00 CaCO3 Aragonite 0.000000000000000E+00
0.000000000000000E+00 K2SO4 Arcanite 0.000000000000000E+00
0.000000000000000E+00 MgCl2.6H2O Bischofite 0.000000000000000E+00
0.000000000000000E+00 Na2Mg (SO4) 2.4H2O Bloedite 0.000000000000000E+00
0.000000000000000E+00 Mg (OH) 2 Brucite 0.000000000000000E+00
0.000000000000000E+00 Na6CO3 (SO4) 2 Burkeite 0.000000000000000E+00
```


Figure 6.5.4 Listing of the Input File FMT_AMPO4_SO4_BM2.INGUESS
(Page 2 of 2)

0.0000000000000000E+00	CaCO3	Calcite	0.0000000000000000E+00
0.0000000000000000E+00	CaCl2.4H2O	CaCl2 Tetrahydrate	0.0000000000000000E+00
0.0000000000000000E+00	Ca4Cl2(OH)6.13H2O	CaOxychloride A	0.0000000000000000E+00
0.0000000000000000E+00	Ca2Cl2(OH)2.H2O	CaOxychloride B	0.0000000000000000E+00
0.0000000000000000E+00	KMgCl3.6H2O	Carnallite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.7H2O	Epsomite	0.0000000000000000E+00
0.0000000000000000E+00	CaNa2(CO3)2.5H2O	Gaylussite	0.0000000000000000E+00
0.0000000000000000E+00	Na2Ca(SO4)2	Glauberite	0.0000000000000000E+00
0.0000000000000000E+00	CaSO4.2H2O	Gypsum	0.0000000000000000E+00
0.0000000000000000E+00	NaCl	Halite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.6H2O	Hexahydrate	0.0000000000000000E+00
0.0000000000000000E+00	KMgClSO4.3H2O	Kainite	0.0000000000000000E+00
0.0000000000000000E+00	KHCO3	Kalcanite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.H2O	Kieserite	0.0000000000000000E+00
0.0000000000000000E+00	K2Mg(SO4)2.4H2O	Leonite	0.0000000000000000E+00
0.0000000000000000E+00	Na4Ca(SO4)3.2H2O	Labile Salt	0.0000000000000000E+00
0.0000000000000000E+00	MgCO3	Magnesite	0.0000000000000000E+00
0.0000000000000000E+00	Mg2Cl(OH)3.4H2O	MgOxychloride	0.0000000000000000E+00
0.0000000000000000E+00	KHSO4	Mercallite	0.0000000000000000E+00
0.0000000000000000E+00	Na2SO4.10H2O	Mirabilite	0.0000000000000000E+00
0.0000000000000000E+00	K8H6(SO4)7	Misenite	0.0000000000000000E+00
0.0000000000000000E+00	NaHCO3	Nahcolite	0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.10H2O	Natron	0.0000000000000000E+00
0.0000000000000000E+00	MgCO3.3H2O	Nesquehonite	0.0000000000000000E+00
0.0000000000000000E+00	K2Mg(SO4)2.6H2O	Picromerite/Schoen	0.0000000000000000E+00
0.0000000000000000E+00	Na2Ca(CO3)2.2H2O	Pirssonite	0.0000000000000000E+00
0.0000000000000000E+00	K2MgCa2(SO4)4.2H2O	Polyhalite	0.0000000000000000E+00
0.0000000000000000E+00	Ca(OH)2	Portlandite	0.0000000000000000E+00
0.0000000000000000E+00	K2CO3.3/2H2O	Potassium Carbonate	0.0000000000000000E+00
0.0000000000000000E+00	K8H4(CO3)6.3H2O	K-Sequicarbonate	0.0000000000000000E+00
0.0000000000000000E+00	KNaCO3.6H2O	K-Na-Carbonate	0.0000000000000000E+00
0.0000000000000000E+00	K2NaH(CO3)2.2H2O	Potassium Trona	0.0000000000000000E+00
0.0000000000000000E+00	K3H(SO4)2	Sesquipotassium Sulfate	0.0000000000000000E+00
0.0000000000000000E+00	Na3H(SO4)2	Sesquisodium Sulfate	0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.7H2O	Na2CO3-Heptahydrate	0.0000000000000000E+00
0.0000000000000000E+00	KCl	Sylvite	0.0000000000000000E+00
0.0000000000000000E+00	K2Ca(SO4)2.H2O	Syngenite	0.0000000000000000E+00
0.0000000000000000E+00	Mg2CaCl6.12H2O	Tachyhydrite	0.0000000000000000E+00
7.586d-2	0.0000000000000000E+00	Na2SO4	Thenardite 0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.H2O	Thermonatrite	0.0000000000000000E+00
0.0000000000000000E+00	Na3H(CO3)2.2H2O	Trona	0.0000000000000000E+00
0.0000000000000000E+00	Na2B4O7.10H2O	Borax	0.0000000000000000E+00
0.0000000000000000E+00	B(OH)3	Borix Acid Solid	0.0000000000000000E+00
0.0000000000000000E+00	KB5O8.4H2O	K-Pentaborate (30_C)	0.0000000000000000E+00
0.0000000000000000E+00	K2B4O7.4H2O	K-Tetraborate (30_C)	0.0000000000000000E+00
0.0000000000000000E+00	NaBO2.4H2O	Sodium Metaborate	0.0000000000000000E+00
0.0000000000000000E+00	NaB5O8.5H2O	Sodium Pentaborate	0.0000000000000000E+00
0.0000000000000000E+00	NaBO2.NaCl.2H2O	Teepelite (20_C)	0.0000000000000000E+00

Figure 6.5.5 Edited Listing of the Output File FMT_AMPO4_SO4_BM1_QB0204.OUT
(Page 1 of 4)

INPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMPO4_SO4_BM1.IN:1
 INGRESS file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMPO4_SO4_BM1.INGRESS:1
 OUTPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMPO4_SO4_BM1_QB0204.OUT:1
 CHEMDAT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT:1
 Temperature Is Hard Coded as 298.15K
 Fig 5, Rai et al 1994, AmPO4(c) Solubility in 10⁻³-3.06 M SO4= Media FMT V2.4
 FMT pH 970407.chemdat
 Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5=== by analogy

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	7.35130E-01	3.91452E-01	0.5325	5.55087E+01	4.91146E+01	8.84809E+05
H+	H+	1.00000E+01	1.27367E+02	12.74	1.00000E+01	8.84809E+00	8.91799E+03
Cl-	Cl-	1.00000E+01	1.27367E+02	12.74	1.00000E+01	8.84809E+00	3.13691E+05
OH-	OH-	3.33355E-16	3.09714E-17	9.2908E-02	3.33355E-16	2.94956E-16	5.10164E-12

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99941E-01	9.99943E-01	1.000	5.55087E+01	5.55587E+01	1.00090E+06
AmPO4(c)	AmPO4(c)	1.00000E+01	1.00000E+00	1.000	1.00000E+01	1.00090E+01	3.38276E+06
Na+	Na+	2.05820E-03	1.94037E-03	0.9428	2.05820E-03	2.06006E-03	4.73602E+01
SO4=	SO4=	8.70692E-04	6.85039E-04	0.7868	8.70692E-04	8.71478E-04	8.37120E+01
H2PO4-	H2PO4-	3.10824E-04	2.91666E-04	0.9384	3.10824E-04	3.11104E-04	3.01731E+01
HPO4=	HPO4=	5.19573E-06	4.09209E-06	0.7876	5.19573E-06	5.20042E-06	4.99134E-01
H+	H+	4.70985E-06	4.43293E-06	0.9412	4.70985E-06	4.71410E-06	4.75134E-03
HSO4-	HSO4-	3.07543E-07	2.89103E-07	0.9400	3.07543E-07	3.07820E-07	2.98787E-02
H3PO4(aq)	H3PO4(aq)	1.80758E-07	1.80714E-07	0.9998	1.80758E-07	1.80921E-07	1.77295E-02
OH-	OH-	2.41912E-09	2.27313E-09	0.9397	2.41912E-09	2.42130E-09	4.11798E-05
Am+++	Am+++	1.71745E-12	3.76073E-13	0.2190	1.71745E-12	1.71900E-12	4.17717E-07
PO4=	PO4=	7.26895E-13	4.19376E-13	0.5769	7.26895E-13	7.27551E-13	6.90967E-08
AmOH++	(after_Cm(III))	3.02077E-17	2.35336E-17	0.7791	3.02077E-17	3.02350E-17	7.86131E-12
Am(OH)2+	(after_Cm(III))	4.12179E-20	3.87867E-20	0.9410	4.12179E-20	4.12550E-20	1.14282E-14
Am(OH)3(aq)	(1e-9m_minimum)	6.99750E-22	6.99750E-22	1.000	6.99750E-22	7.00381E-22	2.05927E-16

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99941E-01	9.99943E-01	1.000	2.06432E+01	5.55587E+01	1.00090E+06
AmPO4(c)	AmPO4(c)	1.00000E+01	1.00000E+00	1.000	3.71891E+00	1.00090E+01	3.38276E+06
Na+	Na+	2.05820E-03	1.94037E-03	0.9428	7.65427E-04	2.06006E-03	4.73602E+01
SO4=	SO4=	8.70692E-04	6.85039E-04	0.7868	3.23803E-04	8.71478E-04	8.37120E+01
H2PO4-	H2PO4-	3.10824E-04	2.91666E-04	0.9384	1.15593E-04	3.11104E-04	3.01731E+01
HPO4=	HPO4=	5.19574E-06	4.09209E-06	0.7876	1.93225E-06	5.20042E-06	4.99134E-01
H+	H+	4.70985E-06	4.43294E-06	0.9412	1.75155E-06	4.71410E-06	4.75134E-03
HSO4-	HSO4-	3.07543E-07	2.89103E-07	0.9400	1.14372E-07	3.07820E-07	2.98787E-02
H3PO4(aq)	H3PO4(aq)	1.80758E-07	1.80714E-07	0.9998	6.72225E-08	1.80921E-07	1.77294E-02
OH-	OH-	2.41912E-09	2.27313E-09	0.9397	8.99651E-10	2.42130E-09	4.11798E-05
Am+++	Am+++	1.71745E-12	3.76073E-13	0.2190	6.38705E-13	1.71900E-12	4.17717E-07
PO4=	PO4=	7.26896E-13	4.19377E-13	0.5769	2.70326E-13	7.27552E-13	6.90967E-08
AmOH++	(after_Cm(III))	3.02077E-17	2.35336E-17	0.7791	1.12340E-17	3.02350E-17	7.86131E-12
Am(OH)2+	(after_Cm(III))	4.12179E-20	3.87867E-20	0.9410	1.53286E-20	4.12550E-20	1.14282E-14
Am(OH)3(aq)	(1e-9m_minimum)	6.99750E-22	6.99750E-22	1.000	2.60231E-22	7.00381E-22	2.05927E-16

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99933E-01	9.99936E-01	1.000	2.06437E+01	5.55586E+01	1.00090E+06
AmPO4(c)	AmPO4(c)	9.99976E+00	1.00000E+00	1.000	3.71891E+00	1.00087E+01	3.38267E+06
Na+	Na+	2.05815E-03	1.93699E-03	0.9411	7.65427E-04	2.06000E-03	4.73589E+01
SO4=	SO4=	8.57205E-04	6.68955E-04	0.7804	3.18795E-04	8.57975E-04	8.24150E+01
H2PO4-	H2PO4-	3.07897E-04	2.88428E-04	0.9368	1.14507E-04	3.08174E-04	2.98890E+01
Cl-	Cl-	2.37916E-04	2.23239E-04	0.9383	8.84809E-05	2.38129E-04	8.44240E+00
H+	H+	2.16061E-04	2.03030E-04	0.9397	8.03532E-05	2.16255E-04	2.17964E-01
HSO4-	HSO4-	1.37747E-05	1.29301E-05	0.9387	5.12281E-06	1.37871E-05	1.33825E+00
H3PO4(aq)	H3PO4(aq)	8.18589E-06	8.18489E-06	0.9999	3.04433E-06	8.19324E-06	8.02899E-01
HPO4=	HPO4=	1.13104E-07	8.83547E-08	0.7812	4.20635E-08	1.13206E-07	1.08655E-02
Am+++	Am+++	3.52028E-09	7.97730E-10	0.2266	1.30919E-09	3.52344E-09	1.56196E-04
OH-	OH-	5.29119E-11	4.96309E-11	0.9380	1.96780E-11	5.29595E-11	9.00697E-07
AmOH++	(after_Cm(III))	1.40872E-15	1.08993E-15	0.7737	5.23902E-16	1.40998E-15	3.66606E-10
PO4=	PO4=	3.50127E-16	1.97706E-16	0.5647	1.30212E-16	3.50441E-16	3.32820E-11
Am(OH)2+	(after_Cm(III))	4.17652E-20	3.92214E-20	0.9386	1.55399E-20	4.18227E-20	1.15855E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99929E-01	9.99932E-01	1.000	2.06439E+01	5.55585E+01	1.00090E+06
AmPO4(c)	AmPO4(c)	9.99965E+00	1.00000E+00	1.000	3.71891E+00	1.00086E+01	3.38263E+06
Na+	Na+	2.05813E-03	1.93532E-03	0.9403	7.65427E-04	2.05997E-03	4.73583E+01
SO4=	SO4=	8.50741E-04	6.61233E-04	0.7772	3.16394E-04	8.51504E-04	8.17935E+01
Cl-	Cl-	3.53176E-04	3.31128E-04	0.9376	1.31348E-04	3.53493E-04	2.5324E+01
H+	H+	3.21015E-04	3.01410E-04	0.9389	1.19387E-04	3.21303E-04	3.23841E-01
H2PO4-	H2PO4-	3.04128E-04	2.84653E-04	0.9360	1.13107E-04	3.04401E-04	2.95231E+01
HSO4-	HSO4-	2.02281E-05	1.89739E-05	0.9380	7.52291E-06	2.02462E-05	1.96521E+00
H3PO4(aq)	H3PO4(aq)	1.19926E-05	1.19919E-05	0.9999	4.46010E-06	1.20033E-05	1.17627E+00
HPO4=	HPO4=	7.54951E-08	5.87369E-08	0.7780	2.80770E-08	7.55628E-08	7.25248E-03

Figure 6.5.5 Edited Listing of the Output File FMT_AMPO4_SO4_BM1_QB0204.OUT
(Page 2 of 4)

Am+++	Am+++	7.73678E-09	1.78144E-09	0.2303	2.87734E-09	7.74372E-09	1.88172E-03	2.31E-09
OH-	OH-	3.56732E-11	3.34313E-11	0.9372	1.32670E-11	3.57052E-11	6.07249E-07	-7.08E-09
AmOH++	(after_Cm(III))	2.12637E-15	1.63952E-15	0.7710	7.90808E-16	2.12828E-15	5.53369E-10	-3.50E-09
PO4--	PO4--	1.58451E-16	8.85329E-17	0.5587	5.89285E-17	1.58593E-16	1.50618E-11	-3.35E-09
Am(OH)2+	(after_Cm(III))	4.23920E-20	3.97412E-20	0.9375	1.57658E-20	4.24301E-20	1.17537E-14	-1.06E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99923E-01	9.99926E-01	1.000	2.06443E+01	5.55584E+01	1.00089E+06
AmPO4 (c)	AmPO4 (c)	9.99948E+00	1.00000E+00	1.000	3.71891E+00	1.00084E+01	3.38256E+06
Na+	Na+	2.05809E-03	1.93287E-03	0.9392	7.65427E-04	2.05993E-03	4.73574E+01
SO4=	SO4=	8.41390E-04	6.50111E-04	0.7727	3.12922E-04	8.42143E-04	8.08942E+01
Cl-	Cl-	5.24272E-04	4.90976E-04	0.9365	1.94982E-04	5.24741E-04	1.86036E+01
H+	H+	4.77258E-04	4.47580E-04	0.9378	1.77497E-04	4.77685E-04	4.81459E-01
H2PO4-	H2PO4-	2.98684E-04	2.79206E-04	0.9348	1.11084E-04	2.98952E-04	2.89945E+01
HSO4-	HSO4-	2.95641E-05	2.77015E-05	0.9370	1.09952E-05	2.95906E-05	2.87223E+00
H3PO4 (aq)	H3PO4 (aq)	1.74660E-05	1.74666E-05	1.000	6.49578E-06	1.74816E-05	1.71311E+00
HPO4=	HPO4=	5.01631E-08	3.87976E-08	0.7734	1.86562E-08	5.02080E-08	4.81894E-03
Am+++	Am+++	1.70155E-08	4.00489E-09	0.2354	6.32824E-09	1.70307E-08	4.13846E-03
OH-	OH-	2.40544E-11	2.25132E-11	0.9359	8.94609E-12	2.40759E-11	4.09466E-07
AmOH++	(after_Cm(III))	3.23543E-15	2.48211E-15	0.7672	1.20329E-15	3.23833E-15	8.41989E-10
PO4--	PO4--	7.15766E-17	3.93809E-17	0.5502	2.66201E-17	7.16407E-17	6.80383E-12
Am(OH)2+	(after_Cm(III))	4.32981E-20	4.05162E-20	0.9357	1.61030E-20	4.33368E-20	1.20049E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99915E-01	9.99917E-01	1.000	2.06448E+01	5.55582E+01	1.00089E+06
AmPO4 (c)	AmPO4 (c)	9.99922E+00	1.00000E+00	1.000	3.71891E+00	1.00081E+01	3.38245E+06
Na+	Na+	2.05804E-03	1.92933E-03	0.9375	7.65427E-04	2.05987E-03	4.73560E+01
SO4=	SO4=	8.28022E-04	6.34311E-04	0.7661	3.07958E-04	8.28760E-04	7.96087E+01
Cl-	Cl-	7.78249E-04	7.27605E-04	0.9349	2.89447E-04	7.78943E-04	2.76159E+01
H+	H+	7.10076E-04	6.64778E-04	0.9362	2.64092E-04	7.10709E-04	7.16324E-01
H2PO4-	H2PO4-	2.90959E-04	2.71485E-04	0.9331	1.08214E-04	2.91218E-04	2.82445E+01
HSO4-	HSO4-	4.29101E-05	4.01444E-05	0.9355	1.59591E-05	4.29484E-05	4.16880E+00
H3PO4 (aq)	H3PO4 (aq)	2.52208E-05	2.52245E-05	1.000	9.38014E-06	2.52433E-05	2.47373E+00
Am+++	Am+++	3.74969E-08	9.08617E-09	0.2423	1.39459E-08	3.75303E-08	9.11986E-03
HPO4=	HPO4=	3.31234E-08	2.53993E-08	0.7668	1.23193E-08	3.31529E-08	3.18200E-03
OH-	OH-	1.62260E-11	1.51575E-11	0.9341	6.03478E-12	1.62405E-11	2.76207E-07
AmOH++	(after_Cm(III))	4.97837E-15	3.79142E-15	0.7616	1.85156E-15	4.98281E-15	1.29557E-09
PO4--	PO4--	3.22617E-17	1.73578E-17	0.5380	1.19988E-17	3.22904E-17	3.06667E-12
Am(OH)2+	(after_Cm(III))	4.46482E-20	4.16677E-20	0.9332	1.66056E-20	4.46880E-20	1.23792E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99902E-01	9.99905E-01	1.000	2.06456E+01	5.55579E+01	1.00089E+06
AmPO4 (c)	AmPO4 (c)	9.99884E+00	1.00000E+00	1.000	3.71891E+00	1.00077E+01	3.38232E+06
Na+	Na+	2.05796E-03	1.92425E-03	0.9350	7.65427E-04	2.05979E-03	4.73540E+01
Cl-	Cl-	1.15525E-03	1.07747E-03	0.9327	4.29676E-04	1.15627E-03	4.09933E+01
H+	H+	1.05745E-03	9.87554E-04	0.9339	3.93302E-04	1.05839E-03	1.06675E+00
SO4=	SO4=	8.09230E-04	6.12299E-04	0.7566	3.00980E-04	8.09947E-04	7.78016E+01
H2PO4-	H2PO4-	2.80241E-04	2.60793E-04	0.9306	1.04231E-04	2.80490E-04	2.72040E+01
HSO4-	HSO4-	6.16696E-05	5.75665E-05	0.9335	2.29371E-05	6.17243E-05	5.99130E+00
H3PO4 (aq)	H3PO4 (aq)	3.59834E-05	3.59974E-05	1.000	1.33835E-05	3.60153E-05	3.52933E+00
Am+++	Am+++	8.30526E-08	2.08737E-08	0.2513	3.08901E-08	8.31263E-08	2.01997E-02
HPO4=	HPO4=	2.16856E-08	1.64243E-08	0.7574	8.06561E-09	2.17048E-08	2.08322E-03
OH-	OH-	1.09526E-11	1.02032E-11	0.9316	4.07365E-12	1.09623E-11	1.86439E-07
AmOH++	(after_Cm(III))	7.77989E-15	5.86315E-15	0.7536	2.89361E-15	7.78679E-15	2.02462E-09
PO4--	PO4--	1.45010E-17	7.55572E-18	0.5210	5.39340E-18	1.45138E-17	1.37840E-12
Am(OH)2+	(after_Cm(III))	4.66588E-20	4.33749E-20	0.9296	1.73540E-20	4.67002E-20	1.29366E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99882E-01	9.99886E-01	1.000	2.06467E+01	5.55575E+01	1.00088E+06
AmPO4 (c)	AmPO4 (c)	9.99828E+00	1.00000E+00	1.000	3.71891E+00	1.00071E+01	3.38211E+06
Na+	Na+	2.05785E-03	1.91707E-03	0.9316	7.65427E-04	2.05966E-03	4.73510E+01
Cl-	Cl-	1.71484E-03	1.59393E-03	0.9295	6.37844E-04	1.71635E-03	6.08497E+01
H+	H+	1.57655E-03	1.46721E-03	0.9306	5.86406E-04	1.57794E-03	1.59040E+01
SO4=	SO4=	7.83421E-04	5.82441E-04	0.7435	2.91397E-04	7.84110E-04	7.53197E+01
H2PO4-	H2PO4-	2.65816E-04	2.46434E-04	0.9271	9.88717E-05	2.66050E-04	2.58035E+01
HSO4-	HSO4-	8.74298E-05	8.13561E-05	0.9305	3.25200E-05	8.75067E-05	8.49388E+00
H3PO4 (aq)	H3PO4 (aq)	5.05015E-05	5.05369E-05	1.001	1.87843E-05	5.05459E-05	4.95326E+00
Am+++	Am+++	1.85991E-07	4.87594E-08	0.2622	6.91802E-08	1.86194E-07	4.52355E-02
HPO4=	HPO4=	1.40370E-08	1.04462E-08	0.7442	5.22114E-09	1.40749E-08	1.34845E-03
OH-	OH-	7.40091E-12	6.86749E-12	0.9279	2.75281E-12	7.40742E-12	1.25980E-07
AmOH++	(after_Cm(III))	1.24148E-14	9.21825E-15	0.7425	4.61777E-15	1.24258E-14	3.23079E-09
PO4--	PO4--	6.49630E-18	3.23458E-18	0.4979	2.43633E-18	6.50201E-18	6.17506E-13
Am(OH)2+	(after_Cm(III))	4.96525E-20	4.59004E-20	0.9244	1.84685E-20	4.96961E-20	1.37666E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99853E-01	9.99858E-01	1.000	2.06485E+01	5.55569E+01	1.00087E+06
AmPO4 (c)	AmPO4 (c)	9.99745E+00	1.00000E+00	1.000	3.71891E+00	1.00061E+01	3.38179E+06
Cl-	Cl-	2.54543E-03	2.35470E-03	0.9251	9.46863E-04	2.54764E-03	9.03214E+01

Figure 6.5.5 Edited Listing of the Output File FMT_AMPO4_SO4_BM1_QB0204.OUT
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Species	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H+	2.35352E-03	2.17968E-03	0.9261	8.75477E-04	2.35557E-03	2.37417E+00	
Na+	2.05768E-03	1.90711E-03	0.9268	7.65427E-04	2.05946E-03	4.73466E+01	
SO4=	7.49075E-04	5.43369E-04	0.7254	2.78646E-04	7.49726E-04	7.20168E+01	
H2PO4-	2.47175E-04	2.27936E-04	0.9222	9.19456E-05	2.47390E-04	2.39937E+01	
HSO4-	1.21703E-04	1.12754E-04	0.9265	4.52718E-05	1.21809E-04	1.18234E+01	3.83E-09
H3PO4 (aq)	6.93609E-05	6.94419E-05	1.001	2.58013E-05	6.94211E-05	6.80294E+00	1.41E-08
Am+++	4.25264E-07	1.16345E-07	0.7261	1.58192E-07	4.25633E-07	1.03429E-01	-3.34E-08
HPO4=	8.95673E-09	6.50387E-09	0.7261	3.33178E-09	8.96451E-09	8.60409E-04	3.07E-08
OH-	5.00929E-12	4.62259E-12	0.9228	1.86339E-12	5.01364E-12	8.52685E-08	-1.32E-09
AmOH++	(after_Cm(III))	2.03557E-14	1.48056E-14	7.57203E-15	2.03734E-14	5.29722E-09	-3.07E-08
PO4--	2.90036E-18	1.35559E-18	0.4674	1.07889E-18	2.90288E-18	2.75691E-13	2.94E-08
Am(OH)2+	(after_Cm(III))	5.41075E-20	4.96226E-20	2.01272E-20	5.41544E-20	1.50016E-14	-3.20E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.99810E-01	9.99816E-01	1.000	2.06510E+01	5.55560E+01	1.00085E+06	
AmPO4 (c)	9.99622E+00	1.00000E+00	1.000	3.71891E+00	1.00047E+01	3.38132E+06	
C1-	3.77816E-03	3.47239E-03	0.9191	1.40560E-03	3.78138E-03	1.34061E+02	
H+	3.51796E-03	3.23665E-03	0.9200	1.30879E-03	3.52095E-03	3.54877E+00	
Na+	2.05742E-03	1.89361E-03	0.9204	7.65427E-04	2.05918E-03	4.73400E+01	
SO4=	7.05212E-04	4.94548E-04	0.7013	2.62361E-04	7.05813E-04	6.77987E+01	
H2PO4-	2.24347E-04	2.05371E-04	0.9154	8.34642E-05	2.24538E-04	2.17774E+01	
HSO4-	1.65459E-04	1.52388E-04	0.9210	6.15559E-05	1.65600E-04	1.60740E+01	2.38E-09
H3PO4 (aq)	9.27344E-05	9.29071E-05	1.002	3.45002E-05	9.28134E-05	9.09528E+00	1.63E-08
Am+++	1.00641E-06	2.84725E-07	0.2829	3.74418E-07	1.00727E-06	2.44767E-01	-3.21E-08
HPO4=	5.62064E-09	3.94635E-09	0.7021	2.09106E-09	5.62542E-09	5.39925E-04	3.12E-08
OH-	3.39920E-12	3.11290E-12	0.9158	1.26461E-12	3.40210E-12	5.78605E-08	-1.42E-09
AmOH++	(after_Cm(III))	3.45017E-14	2.43996E-14	7.07072E-14	3.45311E-14	8.97833E-09	-3.11E-08
PO4--	1.29204E-18	5.53925E-19	0.4287	4.80679E-19	1.29314E-18	1.22811E-13	3.00E-08
Am(OH)2+	(after_Cm(III))	6.07206E-20	5.50704E-20	2.25900E-20	6.07723E-20	1.68348E-14	-3.26E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.99746E-01	9.99754E-01	1.000	2.06548E+01	5.55546E+01	1.00083E+06	
AmPO4 (c)	9.99439E+00	1.00000E+00	1.000	3.71891E+00	1.00027E+01	3.38062E+06	
C1-	5.60756E-03	5.10940E-03	0.9112	2.08657E-03	5.61220E-03	1.98969E+02	
H+	5.26381E-03	4.80066E-03	0.9120	1.95866E-03	5.26817E-03	5.30979E+00	
Na+	2.05705E-03	1.87580E-03	0.9119	7.65427E-04	2.05875E-03	4.73302E+01	
SO4=	6.52006E-04	4.36912E-04	0.6701	2.42611E-04	6.52546E-04	6.26820E+01	
H2PO4-	1.98282E-04	1.79716E-04	0.9064	7.37808E-05	1.98446E-04	1.92468E+01	
HSO4-	2.18506E-04	1.99683E-04	0.9139	8.13060E-05	2.18687E-04	2.12269E+01	2.48E-09
H3PO4 (aq)	1.20239E-04	1.20588E-04	1.003	4.47410E-05	1.20339E-04	1.17926E+01	1.52E-08
Am+++	2.50208E-06	7.15796E-07	0.2861	9.31025E-07	2.50415E-06	6.08509E-01	-4.60E-08
HPO4=	3.46900E-09	2.32829E-09	0.6712	1.29082E-09	3.47188E-09	3.32229E-04	4.16E-08
OH-	2.31544E-12	2.09861E-12	0.9064	8.61577E-13	2.31763E-12	3.91202E-08	-1.42E-09
AmOH++	(after_Cm(III))	6.06915E-14	4.13537E-14	6.814E-14	2.58333E-14	6.07417E-14	5.7933E-08
PO4--	5.76704E-19	2.20337E-19	0.3821	2.14592E-19	5.77181E-19	5.48158E-14	4.04E-08
Am(OH)2+	(after_Cm(III))	7.04560E-20	6.29239E-20	2.62167E-20	7.05143E-20	1.95335E-14	-4.30E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.99506E-01	9.99525E-01	1.000	2.06604E+01	5.55526E+01	1.00079E+06	
AmPO4 (c)	9.99167E+00	1.00000E+00	1.000	3.71891E+00	9.99588E+00	3.37957E+06	
C1-	8.32202E-03	7.49885E-03	0.9011	3.09746E-03	8.32861E-03	2.95274E+02	
H+	7.87849E-03	7.10470E-03	0.9018	2.93238E-03	7.88473E-03	7.94702E+00	
Na+	2.05649E-03	1.85298E-03	0.9010	7.65427E-04	2.05812E-03	4.73156E+01	
SO4=	5.91304E-04	3.72040E-04	0.6312	2.20084E-04	5.91772E-04	5.68442E+01	
H2PO4-	1.71165E-04	1.53107E-04	0.8945	6.37076E-05	1.71300E-04	1.66139E+01	
HSO4-	2.78971E-04	2.52428E-04	0.9049	1.03833E-04	2.79192E-04	2.70999E+01	1.31E-08
H3PO4 (aq)	1.51367E-04	1.52039E-04	1.004	5.63389E-05	1.51487E-04	1.48450E+01	-5.82E-08
Am+++	6.59652E-06	1.84022E-06	0.2790	2.45523E-06	6.60174E-06	1.60422E+00	-2.63E-07
HPO4=	2.11824E-09	1.34030E-09	0.6327	7.88412E-10	2.11992E-09	2.03469E-04	1.92E-07
OH-	1.58591E-12	1.41791E-12	0.8941	5.90277E-13	1.58716E-12	2.69934E-08	-6.69E-09
AmOH++	(after_Cm(III))	1.10593E-13	7.18308E-14	4.6495E-14	4.11628E-14	2.87777E-08	-1.92E-07
PO4--	2.60667E-19	8.57050E-20	0.3288	9.70205E-20	2.60873E-19	2.47755E-14	1.86E-07
Am(OH)2+	(after_Cm(III))	8.44352E-20	7.38462E-20	3.14269E-20	8.45020E-20	2.34083E-14	-1.99E-07

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.99506E-01	9.99525E-01	1.000	2.06687E+01	5.55496E+01	1.00074E+06	
AmPO4 (c)	9.98763E+00	1.00000E+00	1.000	3.71891E+00	9.99500E+00	3.37803E+06	
C1-	1.23489E-02	1.09744E-02	0.8887	4.59811E-03	1.23580E-02	4.38127E+02	
H+	1.17815E-02	1.04755E-02	0.8891	4.38687E-03	1.17902E-02	1.18834E+01	
Na+	2.05566E-03	1.82457E-03	0.8876	7.65427E-04	2.05717E-03	4.72940E+01	
SO4=	5.26696E-04	3.07662E-04	0.5841	1.96116E-04	5.27085E-04	5.06305E+01	
H3PO4 (aq)	1.87487E-04	1.88751E-04	1.007	6.98111E-05	1.87626E-04	1.83864E+01	
HSO4-	3.43228E-04	3.06828E-04	0.8939	1.27801E-04	3.43481E-04	3.33402E+01	1.06E-08
H2PO4-	1.46623E-04	1.28914E-04	0.8792	5.45951E-05	1.46731E-04	1.42310E+01	-1.28E-07
Am+++	1.83016E-05	4.75144E-06	0.2596	6.81464E-06	1.83515E-05	4.45058E+00	-2.39E-07
HPO4=	1.30429E-09	7.65377E-10	0.5868	4.85653E-10	1.30525E-09	1.25277E-04	8.84E-08
OH-	1.09455E-12	9.61521E-13	0.8785	4.07558E-13	1.09535E-12	1.86291E-08	-3.14E-09
AmOH++	(after_Cm(III))	2.05599E-13	1.25770E-13	6.6117E-14	7.65551E-14	5.34967E-08	-9.12E-08
PO4--	1.22239E-19	3.31933E-20	0.2715	4.55159E-20	1.22329E-19	1.16178E-14	8.40E-08
Am(OH)2+	(after_Cm(III))	1.03114E-19	8.76810E-20	3.83945E-20	1.03190E-19	2.85851E-14	-9.32E-08

Figure 6.5.5 Edited Listing of the Output File FMT_AMPO4_SO4_BM1_QB0204.OUT
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.99294E-01	9.99323E-01	1.000	2.06811E+01	5.55450E+01	1.00065E+06	
AmPO4 (c)	AmPO4 (c)	9.98163E+00	1.00000E+00	1.000	3.71889E+00	9.98817E+00	3.37572E+06	
Cl-	Cl-	1.83206E-02	1.60133E-02	0.8741	6.82578E-03	1.83326E-02	6.49946E+02	
H+	H+	1.75741E-02	1.53594E-02	0.8740	6.54766E-03	1.75856E-02	1.77246E+01	
Na+	Na+	2.05443E-03	1.79009E-03	0.8713	7.65427E-04	2.05577E-03	4.72618E+01	
SO4=	SO4=	4.62861E-04	2.45006E-04	0.5293	1.72450E-04	4.63164E-04	4.4904E+01	
H3PO4 (aq)	H3PO4 (aq)	2.37166E-04	2.39591E-04	1.010	8.83693E-05	2.37341E-04	2.32583E+01	
HSO4-	HSO4-	4.06544E-04	3.56259E-04	0.8812	1.51468E-04	4.06810E-04	3.94872E+01	5.35E-09
H2PO4-	H2PO4-	1.29812E-04	1.11604E-04	0.8597	4.83646E-05	1.29897E-04	1.25984E+01	-7.19E-08
Am+++	Am+++	5.13780E-05	1.17990E-05	0.2296	1.91421E-05	5.14117E-05	1.24930E+01	-1.79E-07
HPO4=	HPO4=	8.46281E-10	4.51915E-10	0.5340	3.15302E-10	8.46835E-10	8.12789E-05	9.01E-08
OH-	OH-	7.63146E-13	6.55648E-13	0.8591	2.84328E-13	7.63646E-13	1.29876E-08	-1.17E-09
AmOH++	(after_Cm(III))	3.74513E-13	2.12964E-13	0.5686	1.39534E-13	3.74758E-13	9.74399E-08	-9.24E-08
Am(OH)2+	(after_Cm(III))	1.23601E-19	1.01239E-19	0.8191	4.60503E-20	1.23681E-19	3.42616E-14	-9.25E-08
PO4=-	PO4=-	6.25075E-20	1.33670E-20	0.2138	2.32887E-20	6.25485E-20	5.94033E-15	8.79E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.98978E-01	9.99025E-01	1.000	2.06994E+01	5.55380E+01	1.00053E+06	
AmPO4 (c)	AmPO4 (c)	9.97269E+00	1.00000E+00	1.000	3.71886E+00	9.97796E+00	3.37227E+06	
Cl-	Cl-	2.71724E-02	2.32998E-02	0.8575	1.01327E-02	2.71867E-02	9.63851E+02	
H+	H+	2.61098E-02	2.23575E-02	0.8563	9.73646E-03	2.61236E-02	2.63300E+01	
Na+	Na+	2.05261E-03	1.74918E-03	0.8522	7.65427E-04	2.05369E-03	4.72139E+01	
HSO4-	HSO4-	4.64450E-04	4.02667E-04	0.8670	1.73196E-04	4.64695E-04	4.51059E+01	
H3PO4 (aq)	H3PO4 (aq)	3.25263E-04	3.30192E-04	1.015	1.21292E-04	3.25435E-04	3.18911E+01	
SO4=	SO4=	4.04183E-04	1.89180E-04	0.4681	1.50722E-04	4.04397E-04	3.88454E+01	-8.09E-09
Am+++	Am+++	1.36435E-04	2.64054E-05	0.1935	5.08774E-05	1.36507E-04	3.31713E+01	-2.39E-07
H2PO4-	H2PO4-	1.26513E-04	1.05664E-04	0.8352	4.71773E-05	1.26580E-04	1.22766E+01	-1.13E-07
HPO4=	HPO4=	6.18105E-10	2.93939E-10	0.4755	2.30494E-10	6.18431E-10	5.93567E-05	1.06E-07
AmOH++	(after_Cm(III))	6.27887E-13	3.27324E-13	0.5213	2.34142E-13	6.28218E-13	1.63341E-07	-1.10E-07
OH-	OH-	5.38776E-13	4.50291E-13	0.8358	2.00912E-13	5.39061E-13	9.74399E-08	-2.22E-09
Am(OH)2+	(after_Cm(III))	1.37096E-19	1.06866E-19	0.7795	5.11237E-20	1.37168E-19	3.79976E-14	-1.11E-07
PO4=-	PO4=-	3.74461E-20	5.97288E-21	0.1595	1.39638E-20	3.74659E-20	3.55819E-15	1.03E-07

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.98511E-01	9.98587E-01	1.000	2.07267E+01	5.55272E+01	1.00033E+06	
AmPO4 (c)	AmPO4 (c)	9.95939E+00	1.00000E+00	1.000	3.71879E+00	9.96271E+00	3.36711E+06	
Cl-	Cl-	4.02837E-02	3.38217E-02	0.8396	1.50417E-02	4.02971E-02	1.42865E+03	
H+	H+	3.86132E-02	3.22926E-02	0.8363	1.44180E-02	3.86260E-02	3.89312E+01	
Na+	Na+	2.04991E-03	1.70180E-03	0.8302	7.65427E-04	2.05059E-03	4.71426E+01	
HSO4-	HSO4-	5.14108E-04	4.37855E-04	0.8517	1.91966E-04	5.14279E-04	4.99188E+01	
H3PO4 (aq)	H3PO4 (aq)	5.01383E-04	5.12681E-04	1.023	1.87214E-04	5.01551E-04	4.91496E+01	
SO4=	SO4=	3.53383E-04	1.42423E-04	0.4030	1.31952E-04	3.53501E-04	3.39564E+01	-5.55E-09
Am+++	Am+++	3.27510E-04	5.12451E-05	0.1565	1.22291E-04	3.27620E-04	7.96115E+01	-1.09E-07
H2PO4-	H2PO4-	1.41053E-04	1.13587E-04	0.8053	5.26684E-05	1.41100E-04	1.36849E+01	-6.96E-08
HPO4=	HPO4=	5.29241E-10	2.18765E-10	0.4134	1.97616E-10	5.29418E-10	5.08132E-05	2.94E-08
AmOH++	(after_Cm(III))	9.33137E-13	4.39610E-13	0.4711	3.48429E-13	9.33448E-13	2.42703E-07	-3.18E-08
OH-	OH-	3.85612E-13	3.11618E-13	0.8081	1.43986E-13	3.85740E-13	6.56040E-09	-2.04E-09
Am(OH)2+	(after_Cm(III))	1.35998E-19	9.93252E-20	0.7303	5.07812E-20	1.36044E-19	3.76861E-14	-3.28E-08
PO4=-	PO4=-	2.74991E-20	3.07769E-21	0.1119	1.02680E-20	2.75083E-20	2.61250E-15	2.63E-08

Total G/RT= -4.62345650E+03

TITRATE file name is WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMPO4_SO4_BM1_QB0204.TITRATE;1

**Figure 6.5.6 Edited Listing of the Output File
 FMT_AMPO4_SO4_BM1_QB0204.TITRATE
 (Page 1 of 2)**

Fig 5, Rai et al 1994, AmPO4(c) Solubility in 10^{-3.06} M SO4= Media

FMT V2.4

FMT_pH_970407.chemdat
 Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5=== by analogy

Titrant Volumes per Grid Block, in milliliters

1	0.000000 mL
2	0.010000 mL
3	0.014845 mL
4	0.022037 mL
5	0.032713 mL
6	0.048561 mL
7	0.072088 mL
8	0.107013 mL
9	0.158859 mL
10	0.235822 mL
11	0.350072 mL
12	0.519673 mL
13	0.771441 mL
14	1.145186 mL
15	1.700000 mL

Titration Results, molal

0)	H2O	Na+	H+	Cl-	SO4=
1)	2.06432E+01	2.05820E-03	4.70985E-06	0.00000E+00	8.70692E-04
2)	2.06437E+01	2.05815E-03	2.16061E-04	2.37916E-04	8.57205E-04
3)	2.06439E+01	2.05813E-03	3.21015E-04	3.53176E-04	8.50741E-04
4)	2.06443E+01	2.05809E-03	4.77258E-04	5.24272E-04	8.41390E-04
5)	2.06448E+01	2.05804E-03	7.10076E-04	7.78249E-04	8.28022E-04
6)	2.06456E+01	2.05796E-03	1.05745E-03	1.15525E-03	8.09230E-04
7)	2.06467E+01	2.05785E-03	1.57655E-03	1.71484E-03	7.83421E-04
8)	2.06485E+01	2.05768E-03	2.35352E-03	2.54543E-03	7.49075E-04
9)	2.06510E+01	2.05742E-03	3.51796E-03	3.77816E-03	7.05212E-04
10)	2.06548E+01	2.05705E-03	5.26381E-03	5.60756E-03	6.52006E-04
11)	2.06604E+01	2.05649E-03	7.87849E-03	8.32202E-03	5.91304E-04
12)	2.06687E+01	2.05566E-03	1.17815E-02	1.23489E-02	5.26696E-04
13)	2.06811E+01	2.05443E-03	1.75741E-02	1.83206E-02	4.62861E-04
14)	2.06994E+01	2.05261E-03	2.61098E-02	2.71724E-02	4.04183E-04
15)	2.07267E+01	2.04991E-03	3.86132E-02	4.02837E-02	3.53383E-04

0)	HSO4-	OH-
1)	3.07543E-07	2.41912E-09
2)	1.37747E-05	5.29119E-11
3)	2.02281E-05	3.56732E-11
4)	2.95641E-05	2.40544E-11
5)	4.29101E-05	1.62260E-11
6)	6.16696E-05	1.09526E-11
7)	8.74298E-05	7.40091E-12
8)	1.21703E-04	5.00929E-12
9)	1.65459E-04	3.39920E-12
10)	2.18506E-04	2.31544E-12
11)	2.78971E-04	1.58591E-12
12)	3.43228E-04	1.09455E-12
13)	4.06544E-04	7.63146E-13
14)	4.64450E-04	5.38776E-13
15)	5.14108E-04	3.85612E-13

0)	H3PO4 (aq)	H2PO4-	HPO4=	PO4=-	Am+++
1)	1.80758E-07	3.10824E-04	5.19574E-06	7.26896E-13	1.71745E-12
2)	8.18588E-06	3.07897E-04	1.13104E-07	3.50127E-16	3.52028E-09
3)	1.19926E-05	3.04128E-04	7.54951E-08	1.58451E-16	7.73678E-09
4)	1.74660E-05	2.98684E-04	5.01631E-08	7.15766E-17	1.70155E-08
5)	2.52208E-05	2.90959E-04	3.31234E-08	3.22617E-17	3.74969E-08
6)	3.59834E-05	2.80241E-04	2.16856E-08	1.45010E-17	8.30526E-08

Figure 6.5.6 Edited Listing of the Output File FMT_
AMPO4_SO4_BM1_QB0204.TITRATE
 (Page 2 of 2)

7)	5.05015E-05	2.65816E-04	1.40370E-08	6.49630E-18	1.85991E-07	
8)	6.93609E-05	2.47175E-04	8.95673E-09	2.90036E-18	4.25264E-07	9) 9.27344E-05
	2.24347E-04	5.62064E-09	1.29204E-18	1.00641E-06		
10)	1.20239E-04	1.98282E-04	3.46900E-09	5.76704E-19	2.50208E-06	
11)	1.51367E-04	1.71165E-04	2.11824E-09	2.60667E-19	6.59652E-06	
12)	1.87487E-04	1.46623E-04	1.30429E-09	1.22239E-19	1.83016E-05	
13)	2.37186E-04	1.29812E-04	8.46281E-10	6.25075E-20	5.13780E-05	
14)	3.25263E-04	1.26513E-04	6.18105E-10	3.74461E-20	1.36435E-04	
15)	5.01383E-04	1.41053E-04	5.29241E-10	2.74991E-20	3.27510E-04	
0)	AmOH++	Am(OH) 2+	Am(OH) 3 (aq)			
1)	3.02077E-17	4.12179E-20	6.99750E-22			
2)	1.40872E-15	4.17852E-20				
3)	2.12637E-15	4.23920E-20				
4)	3.23543E-15	4.32981E-20				
5)	4.97837E-15	4.46482E-20				
6)	7.77989E-15	4.66588E-20				
7)	1.24148E-14	4.96525E-20				
8)	2.03557E-14	5.41075E-20				
9)	3.45017E-14	6.07206E-20				
10)	6.06915E-14	7.04560E-20				
11)	1.10593E-13	8.44352E-20				
12)	2.05599E-13	1.03114E-19				
13)	3.74513E-13	1.23601E-19				
14)	6.27887E-13	1.37096E-19				
15)	9.33137E-13	1.35998E-19				
0)	AmPO4 (c)					
1)	1.00000E+01					
2)	9.99976E+00					
3)	9.99965E+00					
4)	9.99948E+00					
5)	9.99922E+00					
6)	9.99884E+00					
7)	9.99828E+00					
8)	9.99745E+00					
9)	9.99622E+00					
10)	9.99439E+00					
11)	9.99167E+00					
12)	9.98763E+00					
13)	9.98163E+00					
14)	9.97269E+00					
15)	9.95939E+00					
0)	IonicStrength	Titrvol,ml	pH	pmH		
1)	2.93880E-03	0.000000000E+00	5.353	5.327		
2)	3.13155E-03	1.000000000E-02	3.692	3.665		
3)	3.23001E-03	1.484475362E-02	3.521	3.493		
4)	3.37689E-03	2.203667100E-02	3.349	3.321		
5)	3.59640E-03	3.271289516E-02	3.177	3.149		
6)	3.92516E-03	4.856148689E-02	3.005	2.976		
7)	4.41895E-03	7.208833083E-02	2.834	2.802		
8)	5.16283E-03	0.107013351	2.662	2.628		
9)	6.28664E-03	0.158858683	2.490	2.454		
10)	7.98788E-03	0.235821801	2.319	2.279		
11)	1.05659E-02	0.350071653	2.148	2.104		
12)	1.44737E-02	0.519672744	1.980	1.929		
13)	2.03997E-02	0.771441385	1.814	1.755		
14)	2.93852E-02	1.14518573	1.651	1.583		
15)	4.29815E-02	1.70000000	1.491	1.413		

Figure 6.5.7 Edited Listing of the Output File FMT_AMPO4_SO4_BM2_QB0204.OUT
(Page 1 of 4)

INPUT file name is:WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMPO4_SO4_BM2.IN;1
 INGUESS file name is:WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMPO4_SO4_BM2.INGUESS;1
 OUTPUT file name is:WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMPO4_SO4_BM2_QB0204.OUT;1
 CHEMDAT file name is WPSNONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
 Temperature is Hard Coded as 298.15K
 Fig 5, Rei et al 1994, AmPO4(c) Solubility in 10^-1.12 M SO4= Media FMT V2.4
 FMT_ph_970407.chemdat
 Added Th(CO3)5-C1(-Na) Parns, assigned K+-Th(CO3)5=== by analogy

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	7.35130E-01	3.91452E-01	0.5325	5.55087E+01	4.91146E+01	8.84809E+05	
H+	H+	1.00000E+01	1.27367E+02	12.74	1.00000E+01	8.84809E+00	8.91799E+03	
Cl-	Cl-	1.00000E+01	1.27367E+02	12.74	1.00000E+01	8.84809E+00	3.13691E+05	
OH-	OH-	3.33355E-16	3.09714E-17	9.2908E-02	3.33355E-16	2.94956E-16	5.01640E-12	-2.45E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95905E-01	9.96680E-01	1.001	5.55087E+01	5.53465E+01	9.97078E+05	
AmPO4(c)	AmPO4(c)	1.00000E+01	1.00000E+00	1.000	1.00000E+01	9.97078E+00	3.36984E+06	
Na+	Na+	1.52036E-01	1.09641E-01	0.7212	1.52036E-01	1.51592E-01	3.48507E+03	
SO4=	SO4=	7.58515E-02	1.69768E-02	0.2238	7.58515E-02	7.56298E-02	7.26482E+03	
H2PO4-	H2PO4-	3.02078E-04	1.87918E-04	0.6221	3.02078E-04	3.01195E-04	2.92121E+01	
HPO4=	HPO4=	1.40278E-05	3.25158E-06	0.2318	1.40278E-05	1.39868E-05	1.34245E+00	
HSO4-	HSO4-	8.54393E-06	5.80937E-06	0.6799	8.54393E-06	8.51897E-06	8.26898E-01	2.34E-07
H+	H+	5.39348E-06	3.59440E-06	0.6664	5.39348E-06	5.37772E-06	5.42020E-03	-1.04E-08
H3PO4(aq)	H3PO4(aq)	9.44308E-08	9.44083E-08	0.9998	9.44308E-08	9.41549E-08	9.22674E-03	2.21E-07
OH-	OH-	4.16485E-09	2.79428E-09	0.6709	4.16485E-09	4.15268E-09	7.06259E-05	-2.17E-07
Am+++	Am+++	7.00595E-11	3.83757E-13	5.4776E-03	7.00595E-11	6.98548E-11	1.69747E-05	4.25E-07
PO4=-	PO4=-	1.05318E-11	4.10979E-13	3.9023E-02	1.05318E-11	1.05011E-11	9.97303E-07	-4.25E-07
AmOH++	(after_Cm(III))	1.73987E-16	2.95202E-17	0.1697	1.73987E-16	1.73479E-16	4.51057E-11	2.08E-07
Am(OH)2+	(after_Cm(III))	9.11755E-20	5.98080E-20	0.6560	9.11755E-20	9.09092E-20	2.51832E-14	-9.98E-09
Am(OH)3(aq)	(1e-9m_minimum)	1.32637E-21	1.32637E-21	1.000	1.32637E-21	1.32250E-21	3.88843E-16	-2.28E-07

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95905E-01	9.96680E-01	1.001	2.06138E+01	5.53465E+01	9.97078E+05	
AmPO4(c)	AmPO4(c)	1.00000E+01	1.00000E+00	1.000	3.71362E+00	9.97078E+00	3.36984E+06	
Na+	Na+	1.52036E-01	1.09641E-01	0.7212	5.64605E-02	1.51592E-01	3.48507E+03	
SO4=	SO4=	7.58515E-02	1.69768E-02	0.2238	2.81684E-02	7.56298E-02	7.26482E+03	
H2PO4-	H2PO4-	3.02078E-04	1.87918E-04	0.6221	1.12180E-04	3.01195E-04	2.92121E+01	
HPO4=	HPO4=	1.40278E-05	3.25158E-06	0.2318	5.20939E-06	1.39868E-05	1.34245E+00	
HSO4-	HSO4-	8.54393E-06	5.80937E-06	0.6799	3.17289E-06	8.51897E-06	8.26898E-01	2.69E-08
H+	H+	5.39348E-06	3.59440E-06	0.6664	2.00293E-06	5.37772E-06	5.42020E-03	-1.27E-07
H3PO4(aq)	H3PO4(aq)	9.44308E-08	9.44082E-08	0.9998	3.50680E-08	9.41549E-08	9.22673E-03	-1.07E-07
OH-	OH-	4.16485E-09	2.79428E-09	0.6709	1.54667E-09	4.15268E-09	7.06259E-05	1.04E-07
Am+++	Am+++	7.00594E-11	3.83757E-13	5.4776E-03	2.60174E-11	6.98547E-11	1.69747E-05	-2.04E-07
PO4=-	PO4=-	1.05318E-11	4.10979E-13	3.9023E-02	3.91113E-12	1.05011E-11	9.97304E-07	2.04E-07
AmOH++	(after_Cm(III))	1.73987E-16	2.95202E-17	0.1697	6.46121E-17	1.73478E-16	4.51057E-11	-9.98E-08
Am(OH)2+	(after_Cm(III))	9.11755E-20	5.98080E-20	0.6560	3.38592E-20	9.09092E-20	2.51832E-14	4.72E-09
Am(OH)3(aq)	(1e-9m_minimum)	1.32637E-21	1.32637E-21	1.000	4.92565E-22	1.32250E-21	3.88843E-16	1.09E-07

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95900E-01	9.96674E-01	1.001	2.06143E+01	5.53463E+01	9.97075E+05	
AmPO4(c)	AmPO4(c)	9.99976E+00	1.00000E+00	1.000	3.71362E+00	9.97052E+00	3.36975E+06	
Na+	Na+	1.52036E-01	1.09646E-01	0.7212	5.64605E-02	1.51588E-01	3.48497E+03	
SO4=	SO4=	7.57128E-02	1.69471E-02	0.2238	2.81175E-02	7.54913E-02	7.25151E+03	
H2PO4-	H2PO4-	3.13685E-04	1.95177E-04	0.6222	1.16494E-04	3.12768E-04	3.03345E+01	
Cl-	Cl-	2.38255E-04	1.60522E-04	0.6737	8.84809E-05	2.37558E-04	8.42214E+00	
HSO4-	HSO4-	1.45438E-04	9.89124E-05	0.6801	5.40113E-05	1.45012E-04	1.40757E+01	
H+	H+	9.19595E-05	6.13070E-05	0.6667	3.41511E-05	9.16906E-05	9.24149E-02	3.00E-08
H3PO4(aq)	H3PO4(aq)	1.67278E-06	1.67245E-06	0.9998	6.21224E-07	1.66789E-06	1.63446E-01	8.40E-08
HPO4=	HPO4=	8.54156E-07	1.98003E-07	0.2318	3.17209E-07	8.51658E-07	8.17417E-02	-5.96E-08
Am+++	Am+++	1.95648E-08	1.07489E-10	5.4940E-03	7.26581E-09	1.95076E-08	4.74034E-03	1.25E-07
OH-	OH-	2.44150E-10	1.63826E-10	0.6710	9.06701E-11	2.43436E-10	4.14018E-06	-6.74E-08
PO4=-	PO4=-	3.76183E-14	1.46726E-15	3.9004E-02	1.39703E-14	3.75082E-14	3.56222E-09	-1.24E-07
AmOH++	(after_Cm(III))	2.85516E-15	4.84775E-16	0.1698	1.06032E-15	2.84681E-15	7.40190E-10	5.67E-08
Am(OH)2+	(after_Cm(III))	8.78222E-20	5.75829E-20	0.6557	3.26146E-20	8.75654E-20	2.42569E-14	-1.07E-08

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95897E-01	9.96671E-01	1.001	2.06146E+01	5.53463E+01	9.97074E+05	
AmPO4(c)	AmPO4(c)	9.99964E+00	1.00000E+00	1.000	3.71362E+00	9.97038E+00	3.36971E+06	
Na+	Na+	1.52031E-01	1.09648E-01	0.7212	5.64605E-02	1.51586E-01	3.48492E+03	
SO4=	SO4=	7.56392E-02	1.69310E-02	0.2238	2.80906E-02	7.54179E-02	7.24446E+03	
Cl-	Cl-	3.58128E-04	2.41309E-04	0.6738	1.33000E-04	3.57080E-04	1.26596E+01	
H2PO4-	H2PO4-	3.13158E-04	1.94867E-04	0.6223	1.16299E-04	3.12241E-04	3.02835E+01	
HSO4-	HSO4-	2.18085E-04	1.48337E-04	0.6802	8.09914E-05	2.17447E-04	2.11066E+01	
H+	H+	1.38016E-04	9.20284E-05	0.6668	5.12559E-05	1.37613E-04	1.38700E-01	4.36E-08
H3PO4(aq)	H3PO4(aq)	2.50697E-06	2.50655E-06	0.9998	9.31029E-07	2.49964E-06	2.44953E-01	4.78E-08
HPO4=	HPO4=	5.68103E-07	1.31695E-07	0.2318	2.10980E-07	5.66441E-07	5.43667E-02	-1.50E-08
Am+++	Am+++	4.40850E-08	2.42593E-10	5.5028E-03	1.63721E-08	4.39560E-08	1.06813E-02	2.41E-08

Figure 6.5.7 Edited Listing of the Output File FMT_AMPO4_SO4_BM2_QB0204.OUT
(Page 2 of 4)

OH-	OH-	1.62636E-10	1.09137E-10	0.6710	6.03990E-11	1.62160E-10	2.75790E-06	-1.28E-08
PO4--	PO4--	1.66725E-14	6.50126E-16	3.8994E-02	6.19177E-15	1.66237E-14	1.57878E-09	-2.08E-08
AmOH++	(after_Cm(III))	4.29125E-15	7.28855E-16	0.1698	1.59366E-15	4.27869E-15	1.11249E-09	7.99E-09
Am(OH)2+	(after_Cm(III))	8.79813E-20	5.76741E-20	0.6555	3.26741E-20	8.77239E-20	2.43008E-14	-4.77E-09

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95892E-01	9.96666E-01	1.001	2.06149E+01	5.53461E+01	9.97072E+05
AmPO4(c)	AmPO4(c)	9.99946E+00	1.00000E+00	1.000	3.71362E+00	9.97018E+00	3.69646E+06
Na+	Na+	1.52028E-01	1.09652E-01	0.7213	5.64605E-02	1.51583E-01	3.48485E+03
SO4=	SO4=	7.55266E-02	1.69068E-02	0.2238	2.80500E-02	7.53074E-02	7.23385E+03
Cl-	Cl-	5.38310E-04	3.62770E-04	0.6739	1.99919E-04	5.36734E-04	1.90288E+01
HSO4-	HSO4-	3.27312E-04	2.22671E-04	0.6803	1.21558E-04	3.26354E-04	3.16777E+01
H2PO4-	H2PO4-	3.12149E-04	1.94267E-04	0.6224	1.15927E-04	3.11235E-04	3.01859E+01
H+	H+	2.07419E-04	1.38343E-04	0.6670	7.70316E-05	2.06811E-04	2.08445E-01
H3PO4(aq)	H3PO4(aq)	3.75687E-06	3.75639E-06	0.9999	1.39524E-06	3.74587E-06	3.67078E-01
HPO4=	HPO4=	3.76740E-07	8.73361E-08	0.2318	1.39915E-07	3.75637E-07	3.60534E-02
Am+++	Am+++	9.96896E-08	5.49004E-10	5.5162E-03	3.70229E-08	9.93976E-08	2.41536E-02
OH-	OH-	1.08178E-10	7.25994E-11	0.6711	4.01755E-11	1.07861E-10	1.83443E-06
PO4--	PO4--	7.35815E-15	2.86806E-16	3.8978E-02	2.73269E-15	7.33660E-15	6.96768E-10
AmOH++	(after_Cm(III))	6.46749E-15	1.09904E-15	0.1699	2.40191E-15	6.44855E-15	1.67667E-09
Am(OH)2+	(after_Cm(III))	8.82825E-20	5.78519E-20	0.6553	3.27866E-20	8.80240E-20	2.43839E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95886E-01	9.96659E-01	1.001	2.06155E+01	5.53459E+01	9.97068E+05
AmPO4(c)	AmPO4(c)	9.99919E+00	1.00000E+00	1.000	3.71362E+00	9.96987E+00	3.69532E+06
Na+	Na+	1.52024E-01	1.09658E-01	0.7213	5.64605E-02	1.51578E-01	3.48475E+03
SO4=	SO4=	7.53625E-02	1.68704E-02	0.2239	2.79891E-02	7.51416E-02	7.21792E+03
Cl-	Cl-	8.09139E-04	5.45404E-04	0.6741	3.00508E-04	8.06767E-04	2.86023E+01
HSO4-	HSO4-	4.91329E-04	3.34339E-04	0.6805	1.82476E-04	4.89888E-04	4.75512E+01
H2PO4-	H2PO4-	3.10527E-04	1.93298E-04	0.6225	1.15327E-04	3.09616E-04	3.00289E+01
H+	H+	3.11983E-04	2.08169E-04	0.6672	1.15868E-04	3.11069E-04	3.13526E-01
H3PO4(aq)	H3PO4(aq)	5.62455E-06	5.62417E-06	0.9999	2.08891E-06	5.60806E-06	5.49563E-01
HPO4=	HPO4=	2.49112E-07	5.77513E-08	0.2318	9.25184E-08	2.48382E-07	2.38396E-02
Am+++	Am+++	2.26027E-07	1.25136E-09	5.5363E-03	8.39448E-08	2.25365E-07	5.47636E-02
OH-	OH-	7.18817E-11	4.82470E-11	0.6712	2.66963E-11	7.16709E-11	1.21893E-06
AmOH++	(after_Cm(III))	9.77313E-15	1.66205E-15	0.1701	3.62967E-15	9.74448E-15	2.53364E-09
PO4--	PO4--	3.23552E-15	1.26036E-16	3.8954E-02	1.20165E-15	3.22604E-15	1.06382E-10
Am(OH)2+	(after_Cm(III))	8.87694E-20	5.81411E-20	0.6550	3.29683E-20	8.85092E-20	2.45183E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95876E-01	9.96649E-01	1.001	2.06163E+01	5.53456E+01	9.97063E+05
AmPO4(c)	AmPO4(c)	9.99878E+00	1.00000E+00	1.000	3.71362E+00	9.96942E+00	3.69398E+06
Na+	Na+	1.52018E-01	1.09666E-01	0.7214	5.64605E-02	1.51571E-01	3.48459E+03
SO4=	SO4=	7.51134E-02	1.68157E-02	0.2239	2.78977E-02	7.48928E-02	7.19403E+03
Cl-	Cl-	1.21621E-03	8.20063E-04	0.6743	4.51709E-04	1.21264E-03	4.29916E+01
HSO4-	HSO4-	7.37328E-04	5.01935E-04	0.6807	2.73849E-04	7.35162E-04	7.13589E+01
H2PO4-	H2PO4-	3.08104E-04	1.91849E-04	0.6227	1.14432E-04	3.07199E-04	2.97944E+01
H+	H+	4.69610E-04	3.13536E-04	0.6677	1.74417E-04	4.68231E-04	4.71930E-01
H3PO4(aq)	H3PO4(aq)	8.40719E-06	8.40741E-06	1.000	3.12249E-06	8.38250E-06	8.21446E-01
Am+++	Am+++	5.13798E-07	2.86014E-09	5.5667E-03	1.90828E-07	5.12289E-07	1.24486E-01
HPO4=	HPO4=	1.64149E-07	3.80562E-08	0.2318	6.09662E-08	1.63667E-07	1.57087E-02
OH-	OH-	4.77150E-11	3.20328E-11	0.6713	1.77217E-11	4.75749E-11	8.09320E-07
AmOH++	(after_Cm(III))	1.48139E-14	2.52218E-15	0.1703	5.50200E-15	1.47704E-14	3.84041E-09
PO4--	PO4--	1.41692E-15	5.51428E-17	3.8917E-02	5.26255E-16	1.41276E-15	1.34172E-10
Am(OH)2+	(after_Cm(III))	8.95067E-20	5.85788E-20	0.6545	3.32435E-20	8.92438E-20	2.47218E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95861E-01	9.96633E-01	1.001	2.06176E+01	5.53452E+01	9.97055E+05
AmPO4(c)	AmPO4(c)	9.99817E+00	1.00000E+00	1.000	3.71362E+00	9.96873E+00	3.69155E+06
Na+	Na+	1.52008E-01	1.09679E-01	0.7215	5.64605E-02	1.51561E-01	3.48435E+03
SO4=	SO4=	7.47404E-02	1.67335E-02	0.2239	2.77608E-02	7.45203E-02	7.15824E+03
Cl-	Cl-	1.28203E-03	1.23322E-03	0.6746	6.78986E-04	1.82265E-03	6.46184E+01
HSO4-	HSO4-	1.10576E-03	7.53189E-04	0.6812	4.10712E-04	1.10250E-03	1.07015E+02
H2PO4-	H2PO4-	3.04666E-04	1.89796E-04	0.6230	1.13162E-04	3.03768E-04	2.94617E+01
H+	H+	7.07498E-04	4.72792E-04	0.6683	2.62786E-04	7.05414E-04	7.10987E-01
H3PO4(aq)	H3PO4(aq)	1.25401E-05	1.25422E-05	1.000	4.65777E-06	1.25032E-05	1.22525E+00
Am+++	Am+++	1.17129E-06	6.57395E-09	5.6126E-03	4.35052E-07	1.16784E-06	2.83785E-01
HPO4=	HPO4=	1.07685E-07	2.49672E-08	0.2319	3.99976E-08	1.07368E-07	1.03052E-02
OH-	OH-	3.16325E-11	2.12425E-11	0.6715	1.17493E-11	3.15394E-11	5.36400E-07
AmOH++	(after_Cm(III))	2.25412E-14	3.84436E-15	0.1705	8.37247E-15	2.24748E-14	5.84361E-09
PO4--	PO4--	6.17346E-16	2.39911E-17	3.8862E-02	2.29301E-16	6.15528E-16	5.84577E-11
Am(OH)2+	(after_Cm(III))	9.05773E-20	5.92106E-20	0.6537	3.36432E-20	9.03106E-20	2.50174E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95838E-01	9.96610E-01	1.001	2.06195E+01	5.53446E+01	9.97043E+05
AmPO4(c)	AmPO4(c)	9.99725E+00	1.00000E+00	1.000	3.71362E+00	9.96769E+00	3.68880E+06
Na+	Na+	1.51994E-01	1.09697E-01	0.7217	5.64605E-02	1.51545E-01	3.48399E+03
SO4=	SO4=	7.41827E-02	1.66103E-02	0.2239	2.75562E-02	7.39634E-02	7.10475E+03

Figure 6.5.7 Edited Listing of the Output File FMT_AMPO4_SO4_BM2_QB0204.OUT
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Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.95804E-01	9.96574E-01	1.001	2.06223E+01	5.53436E+01	9.97025E+05	
AmPO4(c)	9.99586E+00	1.00000E+00	1.000	3.71362E+00	9.96613E+00	3.36827E+06	
Na+	1.51973E-01	1.09723E-01	0.7220	5.64605E-02	1.51521E-01	3.48344E+03	1.33E-08
SO4=	7.33518E-02	1.64257E-02	0.2239	2.72513E-02	7.31336E-02	7.02504E+03	5.74E-08
Cl-	4.12941E-03	2.79098E-03	0.6759	1.53414E-03	4.11713E-03	1.45965E+02	6.75E-08
H2PO4-	2.47686E-03	1.69084E-03	0.6827	9.20194E-04	2.46950E-03	2.39703E+02	7.27E-09
HPO4=	2.94115E-04	1.83720E-04	0.6240	1.09380E-04	2.93539E-04	2.84696E+01	-5.43E-09
H+	1.61258E-03	1.08127E-03	0.6705	5.99097E-04	1.60778E-03	1.62048E+00	-4.96E-08
H3PO4(aq)	2.77461E-05	2.77655E-05	1.001	1.03081E-05	2.76635E-05	2.71090E+00	2.89E-08
Am+++	6.13688E-06	3.55208E-08	5.7881E-03	2.27995E-06	6.11862E-06	4.48683E+00	4.27E-09
HPO4=	4.55732E-08	1.05676E-08	0.2319	1.69312E-08	4.54377E-08	4.36109E-03	-2.87E-08
OH-	1.38155E-11	9.28788E-12	0.6723	5.13266E-12	1.37744E-11	2.34265E-07	-2.32E-08
AmOH++	5.29168E-14	9.08222E-15	0.1716	1.96594E-14	5.27593E-14	1.37178E-08	-2.45E-08
PO4=	1.14898E-16	4.44011E-18	3.8644E-02	4.26862E-17	1.14556E-16	1.08795E-11	
Am(OH)2+	9.39753E-20	6.11616E-20	0.6508	3.49133E-20	9.36957E-20	2.59551E-14	

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.95753E-01	9.96521E-01	1.001	2.06266E+01	5.53421E+01	9.96998E+05	
AmPO4(c)	9.99378E+00	1.00000E+00	1.000	3.71362E+00	9.96378E+00	3.36747E+06	
Na+	1.51942E-01	1.09759E-01	0.7224	5.64605E-02	1.51486E-01	3.48262E+03	1.33E-08
SO4=	7.21196E-02	1.61496E-02	0.2239	2.67991E-02	7.19031E-02	6.90684E+03	5.74E-08
Cl-	6.20584E-03	4.20145E-03	0.6770	2.30605E-03	6.18721E-03	2.19355E+02	6.75E-08
H2PO4-	3.69329E-03	2.52618E-03	0.6840	1.37240E-03	3.68220E-03	3.57414E+02	7.27E-09
HPO4=	2.88640E-04	1.80377E-04	0.6249	1.07256E-04	2.87773E-04	2.79104E+01	-5.43E-09
H+	2.44313E-03	1.64307E-03	0.6725	9.07849E-04	2.43579E-03	2.45504E+00	-4.96E-08
H3PO4(aq)	4.13750E-05	4.14241E-05	1.001	1.53746E-05	4.12508E-05	4.04238E+00	-9.83E-08
Am+++	1.40402E-05	8.35419E-08	5.9502E-03	5.21724E-06	1.39981E-05	3.40153E+00	4.79E-08
HPO4=	2.94459E-08	6.82778E-09	0.2319	1.09419E-08	2.93575E-08	2.81771E-03	2.36E-08
OH-	9.08247E-12	6.11182E-12	0.6729	3.37498E-12	9.05521E-12	1.54005E-07	-4.86E-08
AmOH++	1.14408E-14	1.40056E-14	0.1726	3.02628E-14	8.11963E-14	2.11116E-08	7.37E-08
PO4=	4.91163E-17	1.88787E-18	3.8437E-02	1.82513E-17	4.89689E-17	4.65065E-12	-2.56E-08
Am(OH)2+	9.60927E-20	6.22884E-20	0.6482	3.57074E-20	9.58042E-20	2.65392E-14	

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.95675E-01	9.96440E-01	1.001	2.06331E+01	5.53397E+01	9.96957E+05	
AmPO4(c)	9.99064E+00	1.00000E+00	1.000	3.71361E+00	9.96024E+00	3.36628E+06	
Na+	1.51894E-01	1.09806E-01	0.7229	5.64605E-02	1.51432E-01	3.48139E+03	1.33E-08
SO4=	7.03062E-02	1.57383E-02	0.2239	2.61335E-02	7.00923E-02	6.73289E+03	5.74E-08
Cl-	9.32539E-03	6.32932E-03	0.6787	3.46633E-03	9.29701E-03	3.29670E+02	6.75E-08
H2PO4-	5.48302E-03	3.76120E-03	0.6860	2.03809E-03	5.46633E-03	5.30593E+02	7.27E-09
HPO4=	2.85133E-04	1.78549E-04	0.6262	1.05987E-04	2.84266E-04	2.75702E+01	-5.43E-09
H+	3.71632E-03	2.51028E-03	0.6755	1.38139E-03	3.70501E-03	3.73428E+00	-4.96E-08
H3PO4(aq)	6.25255E-05	6.26461E-05	1.002	2.32413E-05	6.23352E-05	6.10856E+00	-1.15E-07
Am+++	3.17729E-05	1.96997E-07	6.2002E-03	1.18103E-05	3.16762E-05	7.69732E+00	5.09E-08
HPO4=	1.90838E-08	4.42372E-09	0.2318	7.09362E-09	1.90257E-08	1.82608E-03	1.29E-08
OH-	5.93628E-12	4.00009E-12	0.6738	2.20657E-12	5.91821E-12	1.00653E-07	-4.99E-08
AmOH++	1.24669E-13	2.16931E-14	0.1740	4.63404E-14	1.24289E-13	3.23161E-08	6.42E-08
PO4=	2.10101E-17	8.00601E-19	3.8106E-02	7.80964E-18	2.09462E-17	1.98929E-12	-3.76E-08
Am(OH)2+	9.76578E-20	6.29161E-20	0.6443	3.63003E-20	9.73606E-20	2.69703E-14	

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	9.95557E-01	9.96318E-01	1.001	2.06428E+01	5.53362E+01	9.96893E+05	
AmPO4(c)	9.98592E+00	1.00000E+00	1.000	3.71360E+00	9.95489E+00	3.36447E+06	
Na+	1.51823E-01	1.09861E-01	0.7236	5.64605E-02	1.51351E-01	3.47953E+03	1.33E-08
SO4=	6.76687E-02	1.51296E-02	0.2236	2.51649E-02	6.74585E-02	6.47990E+03	5.74E-08
Cl-	1.40109E-02	9.54491E-03	0.6812	5.21042E-03	1.39674E-02	4.95185E+02	6.75E-08
H2PO4-	8.08498E-03	5.56948E-03	0.6889	3.00667E-03	8.05986E-03	7.82334E+02	7.27E-09
HPO4=	2.88218E-04	1.80978E-04	0.6279	1.07184E-04	2.87323E-04	2.78667E+01	-5.43E-09
H+	5.68844E-03	3.86670E-03	0.6797	2.11544E-03	5.67077E-03	5.71557E+00	-4.96E-08
H3PO4(aq)	9.75097E-05	9.78093E-05	1.003	3.62622E-05	9.72067E-05	9.52580E+00	-8.76E-08
Am+++	6.99835E-05	4.61138E-07	6.5892E-03	2.60257E-05	6.97660E-05	1.69531E+01	1.96E-08
HPO4=	1.25709E-08	2.91096E-09	0.2316	4.67493E-09	1.25319E-08	1.20280E-03	3.92E-09
OH-	3.84625E-12	2.59655E-12	0.6751	1.43036E-12	3.83430E-12	6.52110E-08	-1.91E-08
AmOH++	1.87235E-13	3.29626E-14	0.1760	6.96295E-14	1.86653E-13	4.85311E-08	2.37E-08
PO4=	9.10463E-18	3.42015E-19	3.7565E-02	3.38586E-18	9.07634E-18	8.61995E-13	-1.55E-08
Am(OH)2+	9.72329E-20	6.20566E-20	0.6382	3.61593E-20	9.69308E-20	2.68512E-14	

Figure 6.5.7 Edited Listing of the Output File FMT_AMPO4_SO4_BM2_QB0204.OUT
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TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95376E-01	9.96133E-01	1.001	2.06573E+01	5.53307E+01	9.96794E+05
AmPO4 (c)	AmPO4 (c)	9.97881E+00	1.00000E+00	1.000	3.71357E+00	9.94682E+00	3.36174E+06
Na+	Na+	1.51716E-01	1.09910E-01	0.7244	5.64605E-02	1.51230E-01	3.47674E+03
SO4=	SO4=	6.39037E-02	1.42398E-02	0.2228	2.37815E-02	6.36988E-02	6.11875E+03
Cl-	Cl-	2.10456E-02	1.44151E-02	0.6849	7.83204E-03	2.09782E-02	7.43739E+02
HSO4-	HSO4-	1.17967E-02	8.17549E-03	0.6930	4.39009E-03	1.17589E-02	1.14138E+03
H2PO4-	H2PO4-	3.03021E-04	1.90937E-04	0.6301	1.12768E-04	3.02050E-04	2.92950E+01
H+	H+	8.79347E-03	6.03067E-03	0.6858	3.27245E-03	8.76528E-03	8.83453E+00
H3PO4 (aq)	H3PO4 (aq)	1.60162E-04	1.60942E-04	1.005	5.96036E-05	1.59649E-04	1.56448E+01
Am+++	Am+++	1.47657E-04	1.06320E-06	7.2005E-03	5.49499E-05	1.47184E-04	3.57657E+01
HPO4=	HPO4=	8.52867E-09	1.96913E-09	0.2309	3.17391E-09	8.50133E-09	8.15953E-04
OH-	OH-	2.45987E-12	1.66453E-12	0.6767	9.15429E-13	2.45198E-12	4.17016E+08
AmOH++	(after_Cm(III))	2.72300E-13	4.87192E-14	0.1789	1.01335E-13	2.71427E-13	7.05730E-08
PO4--	PO4--	4.04631E-18	1.48341E-19	3.6661E-02	1.50582E-18	4.03334E-18	3.83053E-13
Am(OH)2+	(after_Cm(III))	9.34735E-20	5.87979E-20	0.6290	3.47857E-20	9.31738E-20	2.58105E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.95097E-01	9.95850E-01	1.001	2.06792E+01	5.53223E+01	9.96643E+05
AmPO4 (c)	AmPO4 (c)	9.96810E+00	1.00000E+00	1.000	3.71351E+00	9.93464E+00	3.35762E+06
Na+	Na+	1.51556E-01	1.09910E-01	0.7252	5.64605E-02	1.51047E-01	3.47253E+03
SO4=	SO4=	5.86957E-02	1.29693E-02	0.2210	2.18665E-02	5.84986E-02	5.61924E+03
Cl-	Cl-	3.16013E-02	2.18103E-02	0.6902	1.17727E-02	3.14952E-02	1.11660E+03
HSO4-	HSO4-	1.69246E-02	1.16277E-02	0.6988	6.30508E-03	1.68678E-02	1.63728E+03
H2PO4-	H2PO4-	3.33069E-04	2.10685E-04	0.6326	1.24081E-04	3.31951E-04	3.21950E+01
H+	H+	1.38012E-02	9.57941E-03	0.6941	5.14149E-03	1.37549E-02	1.38635E+01
Am+++	Am+++	2.97789E-04	2.43118E-06	8.1641E-03	1.10938E-04	2.96790E-04	7.21199E+01
H3PO4 (aq)	H3PO4 (aq)	2.79915E-04	2.82090E-04	1.008	1.04280E-04	2.78976E-04	2.73383E+01
HPO4=	HPO4=	5.96919E-09	1.36788E-09	0.2292	2.22376E-09	5.94915E-09	5.70996E-04
OH-	OH-	1.54429E-12	1.04760E-12	0.6784	5.75309E-13	1.53910E-12	2.61760E-08
AmOH++	(after_Cm(III))	3.83737E-13	7.01141E-14	0.1827	1.42957E-13	3.82449E-13	9.94395E-08
PO4--	PO4--	1.84743E-18	6.48723E-20	3.5115E-02	6.88239E-19	1.84122E-18	1.74864E-13
Am(OH)2+	(after_Cm(III))	8.66016E-20	5.32563E-20	0.6150	3.22625E-20	8.63109E-20	2.39094E-14

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Activity	Act Coef	Total Moles	Molarity	mg/liter	Descriptor
H2O	WATER	9.94663E-01	9.95415E-01	1.001	2.07121E+01	5.53093E+01	9.96408E+05
AmPO4 (c)	AmPO4 (c)	9.95199E+00	1.00000E+00	1.000	3.71341E+00	9.91625E+00	3.35141E+06
Na+	Na+	1.51315E-01	1.09754E-01	0.7253	5.64605E-02	1.50772E-01	3.46621E+03
SO4=	SO4=	5.18884E-02	1.12382E-02	0.2166	1.93612E-02	5.17020E-02	4.96637E+03
Cl-	Cl-	4.74261E-02	3.30626E-02	0.6971	1.76962E-02	4.72557E-02	1.67536E+03
HSO4-	HSO4-	2.36119E-02	1.66819E-02	0.7065	8.81034E-03	2.35271E-02	2.28367E+03
Am+++	Am+++	5.83463E-04	5.63317E-06	9.6547E-03	2.17708E-04	5.81367E-04	1.41272E+02
H+	H+	2.21288E-02	1.55920E-02	0.7046	8.25697E-03	2.20493E-02	2.22235E+01
H3PO4 (aq)	H3PO4 (aq)	5.18442E-04	5.24980E-04	1.013	1.93447E-04	5.16580E-04	5.06224E+01
H2PO4-	H2PO4-	3.79716E-04	2.40894E-04	0.6344	1.41684E-04	3.78353E-04	3.66954E+01
HPO4=	HPO4=	4.27032E-09	9.60893E-10	0.2250	1.59339E-09	4.25498E-09	4.60439E-04
OH-	OH-	9.47057E-13	6.43343E-13	0.6793	3.53377E-13	9.43656E-13	1.60490E-08
AmOH++	(after_Cm(III))	5.33201E-13	9.97672E-14	0.1871	1.98954E-13	5.31286E-13	1.38138E-07
PO4--	PO4--	8.62674E-19	2.79978E-20	3.2455E-02	3.21891E-19	8.59575E-19	8.16352E-14
Am(OH)2+	(after_Cm(III))	7.84298E-20	4.65371E-20	0.5934	2.92647E-20	7.81481E-20	2.16482E-14

Total G/RT= -4.63303143E+03

TITRATE file name is WP6NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMPO4_SO4_BM2_QB0204.TITRATE:1

**Figure 6.5.8 Edited Listing of the Output File
 FMT_AMPO4_SO4_BM2_QB0204.TITRATE
 (Page 1 of 2)**

Fig 5, Rai et al 1994, AmPO4(c) Solubility in 10^{-1.12} M SO4= Media
 FMT_ph_970407.chemdat
 Added Th(CO3)5-Cl(-Na) Parmas, assigned K+-Th(CO3)5=== by analogy

FMT V2.4

Titrant Volumes per Grid Block, in milliliters

1	0.000000 mL
2	0.010000 mL
3	0.015031 mL
4	0.022595 mL
5	0.033963 mL
6	0.051052 mL
7	0.076738 mL
8	0.115349 mL
9	0.173387 mL
10	0.260626 mL
11	0.391761 mL
12	0.588875 mL
13	0.885167 mL
14	1.330539 mL
15	2.000000 mL

Titration Results, molal

0)	H2O	Na+	H+	Cl-	SO4=
1)	2.06138E+01	1.52036E-01	5.39348E-06	0.00000E+00	7.58515E-02
2)	2.06143E+01	1.52033E-01	9.19595E-05	2.38255E-04	7.57128E-02
3)	2.06146E+01	1.52031E-01	1.38016E-04	3.58128E-04	7.56392E-02
4)	2.06149E+01	1.52028E-01	2.07419E-04	5.38310E-04	7.55286E-02
5)	2.06155E+01	1.52024E-01	3.11983E-04	8.09139E-04	7.53625E-02
6)	2.06163E+01	1.52018E-01	4.69610E-04	1.21621E-03	7.51134E-02
7)	2.06176E+01	1.52008E-01	7.07498E-04	1.82803E-03	7.47404E-02
8)	2.06195E+01	1.51994E-01	1.06718E-03	2.74755E-03	7.41827E-02
9)	2.06223E+01	1.51973E-01	1.61258E-03	4.12941E-03	7.33518E-02
10)	2.06266E+01	1.51942E-01	2.44313E-03	6.20584E-03	7.21196E-02
11)	2.06331E+01	1.51894E-01	3.71632E-03	9.32539E-03	7.03062E-02
12)	2.06428E+01	1.51823E-01	5.68844E-03	1.40109E-02	6.76687E-02
13)	2.06573E+01	1.51716E-01	8.79347E-03	2.10456E-02	6.39037E-02
14)	2.06792E+01	1.51556E-01	1.38012E-02	3.16013E-02	5.86957E-02
15)	2.07121E+01	1.51315E-01	2.21288E-02	4.74261E-02	5.18884E-02

0)	HSO4-	OH-
1)	8.54393E-06	4.16485E-09
2)	1.45438E-04	2.44150E-10
3)	2.18085E-04	1.62636E-10
4)	3.27312E-04	1.08178E-10
5)	4.91329E-04	7.18817E-11
6)	7.37328E-04	4.77150E-11
7)	1.10576E-03	3.16325E-11
8)	1.65642E-03	2.09327E-11
9)	2.47686E-03	1.38155E-11
10)	3.69329E-03	9.08247E-12
11)	5.48302E-03	5.93628E-12
12)	8.08498E-03	3.84625E-12
13)	1.17967E-02	2.45987E-12
14)	1.69246E-02	1.54429E-12
15)	2.36119E-02	9.47057E-13

0)	H3PO4 (aq)	H2PO4-	HPO4=	PO4=-	Am+++
1)	9.44308E-08	3.02078E-04	1.40278E-05	1.05318E-11	7.00594E-11
2)	1.67278E-06	3.13685E-04	8.54156E-07	3.76183E-14	1.95648E-08
3)	2.50697E-06	3.13158E-04	5.68103E-07	1.66725E-14	4.40850E-08
4)	3.75687E-06	3.12149E-04	3.76740E-07	7.35815E-15	9.96896E-08
5)	5.62455E-06	3.10527E-04	2.49112E-07	3.23552E-15	2.26027E-07
6)	8.40719E-06	3.08104E-04	1.64149E-07	1.41692E-15	5.13798E-07

**Figure 6.5.8 Edited Listing of the Output File
 FMT_AMPO4_SO4_BM2_QB0204.TITRATE
 (Page 2 of 2)**

```

7) 1.25401E-05 3.04666E-04 1.07685E-07 6.17346E-16 1.17129E-06
□
8) 1.86634E-05 3.00058E-04 7.02590E-08 2.67273E-16 2.67819E-06 9) 2.77461E-05
2.94415E-04 4.55732E-08 1.14898E-16 6.13688E-06
10) 4.13750E-05 2.88640E-04 2.94459E-08 4.91163E-17 1.40402E-05
11) 6.25255E-05 2.85133E-04 1.90838E-08 2.10101E-17 3.17729E-05
12) 9.75097E-05 2.88218E-04 1.25709E-08 9.10463E-18 6.99835E-05
13) 1.60162E-04 3.03021E-04 8.52867E-09 4.04631E-18 1.47657E-04
14) 2.79915E-04 3.33069E-04 5.96919E-09 1.84743E-18 2.97789E-04
15) 5.18442E-04 3.79716E-04 4.27032E-09 8.62674E-19 5.83463E-04

0) AmOH++ Am(OH) 2+ Am(OH) 3 (aq)
1) 1.73987E-16 9.11755E-20 1.32637E-21
2) 2.85516E-15 8.78222E-20 0.00000E+00
3) 4.29125E-15 8.79813E-20 0.00000E+00
4) 6.46749E-15 8.82825E-20 0.00000E+00
5) 9.77313E-15 8.87694E-20 0.00000E+00
6) 1.48139E-14 8.95067E-20 0.00000E+00
7) 2.25412E-14 9.05773E-20 0.00000E+00
8) 3.44576E-14 9.20624E-20 0.00000E+00
9) 5.29168E-14 9.39753E-20 0.00000E+00
10) 8.14408E-14 9.60927E-20 0.00000E+00
11) 1.24669E-13 9.76578E-20 0.00000E+00
12) 1.87235E-13 9.72329E-20 0.00000E+00
13) 2.72300E-13 9.34735E-20 0.00000E+00
14) 3.83737E-13 8.66016E-20 0.00000E+00
15) 5.33201E-13 7.84298E-20 0.00000E+00

0) AmPO4 (c)
1) 1.00000E+01
2) 9.99976E+00
3) 9.99964E+00
4) 9.99946E+00
5) 9.99919E+00
6) 9.99878E+00
7) 9.99817E+00
8) 9.99725E+00
9) 9.99586E+00
10) 9.99378E+00
11) 9.99064E+00
12) 9.98592E+00
13) 9.97881E+00
14) 9.96810E+00
15) 9.95199E+00

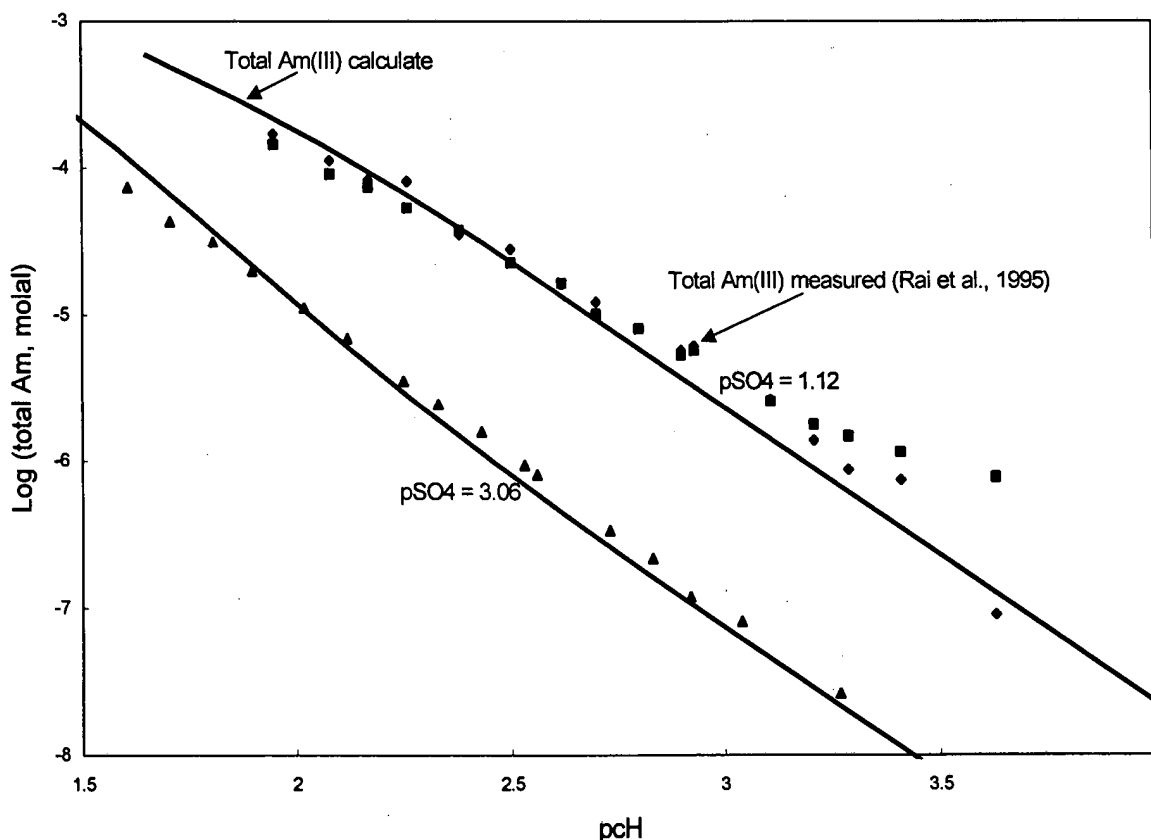
0) IonicStrength Titrvol,ml pH pmH
1) 2.27907E-01 0.000000000E+00 5.444 5.268
2) 2.27838E-01 1.000000000E-02 4.212 4.036
3) 2.27809E-01 1.503149952E-02 4.036 3.860
4) 2.27765E-01 2.259459779E-02 3.859 3.683
5) 2.27700E-01 3.396306858E-02 3.682 3.506
6) 2.27604E-01 5.105158491E-02 3.504 3.328
7) 2.27463E-01 7.673818742E-02 3.325 3.150
8) 2.27260E-01 0.115349003 3.146 2.972
9) 2.26975E-01 0.173386848 2.966 2.792
10) 2.26589E-01 0.260626432 2.784 2.612
11) 2.26108E-01 0.391760609 2.600 2.430
12) 2.25600E-01 0.588874941 2.413 2.245
13) 2.25299E-01 0.885167339 2.220 2.056
14) 2.25839E-01 1.33053924 2.019 1.860
15) 2.28833E-01 2.00000000 1.807 1.655
  
```

6.5.4 Evaluation

The calculated solubility of AmPO_4 was to be graphically compared with the experimental data from Rai et al. (1995) for the solubility of Am(III) in $10^{-3.5}\text{m}$ NaH_2PO_4 media with both $10^{-3.06}\text{m}$ and $10^{-1.12}\text{m}$ Na_2SO_4 as hydrogen ion concentration is changed by the addition of HCl from Rai et al. (1995). The model prediction was to follow the general trend of the experimental data and the deviation of the model prediction from the experimental data was to be less than half logarithmic unit.

Figures 6.5.5 and 6.5.7 show the nonzero concentrations calculated by FMT. Figures 6.5.6 and 6.5.8 show the nonzero titration results from FMT. Figure 6.5.9 is a graph of the comparison of the calculated Am(III) molality with the experimental measurements from Rai et al. (1995). It can be seen that the model prediction follows the general trend of the experimental data and the deviation of the model prediction from the experimental measurements was less than half a logarithmic unit. Therefore, the acceptance criteria is considered to have been met.

Figure 6.5.9 Comparison of the Calculated Am(III) Molality with the Experimental Measurements from Rai et al. (1995)



6.6 Test Case #6: Fixing CO₂ Fugacity or pH and Disabling Chemical Species as Needed

6.6.1 Test Objectives

This test case is a "Batch calculation for the speciation of a Na-K-Cl-CO₂ solution with a fixed pH of 8.3 and f_{CO_2} of 10^{-4} atm. Species NaCl (halite) and CO₂ (aq) are disabled in the calculation. This test case was to demonstrate the capability of the code for fixing CO₂ fugacity or pH and disabling chemical species as specified in the input file. It tests functional requirements R.5, and R.6.

6.6.2 Test Procedures

This test case was run using the script FMT_TEST_QB0204.COM. This command file is shown in **Figure 6.0.2**.

6.6.3 Input/Output Files

The following is a list of all files associated with Test Case #6:

Command file:

FMT_TEST_QB0204.COM

Input files:

FMT_FCO2_PH_FIXED.IN

(See **Figure 6.6.1**)

FMT_FCO2_PH_FIXED.INGUESS

(See **Figure 6.6.2**)

Output files:

FMT_FCO2_PH_FIXED_QB0204.OUT

(See **Figure 6.6.3**)

Figure 6.6.1 Listing of the Input File FMT_FCO2_PH_FIXED.IN

```
'SETTING CO2 fugacity and pH'  
'CHEMFILE'  
'BATCH' 'EXPLICIT'  
'DISABLE_SPECIES' 2  
 171 14  
'SET_FCO2' 0.99999e-4 1.00001d-4  
'SET_ph' 8.3  
  
'nMOLES' 'nEXACT'  
111. Hydrogen  
79.5 Oxygen  
7.0 Sodium  
4.5 Potassium  
0 Magnesium  
0 Calcium  
11.5 Chlorine  
0 Sulfur  
12.0 Carbon  
0.0 PosIon:EL  
0.0 NegIon:EL  
0.0 Oxalate:EL  
0 Boron  
0 Bromine  
0.0 Acetate:EL  
0 Th(IV)  
0 Am(III)  
0.0 U(VI)  
0 Np(V)  
0.0 ClO4:EL  
0.0 Phosphorus  
0.0 U(IV)  
0.0 Lactate:EL  
0.0 EDTA:EL  
0.0 Citrate:EL  
0.0 Electron:E  
0.0 Charge:EL
```

Figure 6.6.2 Listing of the Input File FMT_FCO2_PH_FIXED.INGUESS

(This file is necessary but is intentionally blank for this test case.)

Figure 6.6.3 Edited Listing of the Output File FMT_FCO2_PH_FIXED_QB0204.OUT

INPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_FCO2_PH_FIXED.IN;1
 INGUESS file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_FCO2_PH_FIXED.INGUESS;1
 OUTPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_FCO2_PH_FIXED_QB0204.OUT;
 CHEMDAT file name is WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
 TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Molality	Molarity	mg/liter
□			
□			
H2O	7.66638E-01	4.68417E+01	8.43862E+05
CO2 ("solid", f=9.9999e-05_atm)	1.20013E+01	1.01274E+01	4.45705E+05
Cl- Cl-	8.44793E+00	7.12888E+00	2.52740E+05
Na+ Na+	7.00120E+00	5.90804E+00	1.35825E+05
KCl Sylvite	3.05404E+00	2.57719E+00	1.92133E+05
H+(solid)_pH= 8.30000	8.50389E-04	7.17611E-04	7.23280E-01
K+ K+	1.44673E+00	1.22084E+00	4.77328E+04
HCO3- HCO3-	7.40299E-04	6.24711E-04	3.81180E+01
CO3= CO3=	5.40304E-05	4.55942E-05	2.73607E+00
OH- OH-	2.02952E-06	1.71264E-06	2.91273E-02
H+ H+	5.68031E-10	4.79340E-10	4.83127E-07
Na3H(CO3)2.2H2O Trona	0.00000E+00	0.00000E+00	0.00000E+00
OH-/H2O(solid)_pH= 8.30000	0.00000E+00	0.00000E+00	0.00000E+00
NaCl Halite NAF	0.00000E+00	0.00000E+00	0.00000E+00
KHCO3 Kalicinite	0.00000E+00	0.00000E+00	0.00000E+00
NaHCO3 Nahcolite	0.00000E+00	0.00000E+00	0.00000E+00
Na2CO3.10H2O Natron	0.00000E+00	0.00000E+00	0.00000E+00
K2CO3.3/2H2O Potassium Carbonate	0.00000E+00	0.00000E+00	0.00000E+00
K8H4(CO3)6.3H2O K-Sequicarbonate	0.00000E+00	0.00000E+00	0.00000E+00
KNaCO3.6H2O K-Na-Carbonate	0.00000E+00	0.00000E+00	0.00000E+00
K2NaH(CO3)2.2H2O Potassium Trona	0.00000E+00	0.00000E+00	0.00000E+00
Na2CO3.7H2O Na2CO3-Heptahydrate	0.00000E+00	0.00000E+00	0.00000E+00
Na2CO3.H2O Thermonatrite	0.00000E+00	0.00000E+00	0.00000E+00
CO2(aq) CO2(aq) NAF	0.00000E+00	0.00000E+00	0.00000E+00
NaOH(aq) to.titrate.base.only	0.00000E+00	0.00000E+00	0.00000E+00
HCl(aq) to.titrate.acid.only	0.00000E+00	0.00000E+00	0.00000E+00
pH (-log[aH+]); pM(-log[mH+]); pCH(-log[MH+])	8.3000	9.2456	9.3194
Osmotic Coefficient=	1.391564		
Equilibrium RH (%) =	65.469402		
Ionic Strength (m) =	8.448404		
Density, kg/m3 =	1280.20		
fCO2(g); log[fCO2(g)] =		1.000E-04	-4.000

NOTES: - Water "molality" is mole fraction H2O in aqueous phase
 - "Descriptor" means:
 *dG/RT/ln10 for species with nonzero concs. (convergence criterion)
 *Saturation Index for minerals, SI=log10(IAP/Ksp)
 *log10(activity) for aqueous species with very small concentrations
 *log10(activity) for aqueous species Not Allowed to Form
 *NAF signifies that the species was Not Allowed to Form

6.6.4 Evaluation

In this case, a sufficient quantity of halite is added to the solution, and precipitation of the mineral would occur if it were not disabled. Similarly, the concentration of CO_2 (aq) would be non-zero, if this species were not disabled. Therefore, the calculated concentrations of both NaCl (halite) and CO_2 (aq) must be zero. The calculated pH and f_{CO_2} must be the same, to four significant digits, as those specified in the input file.

An edited listing of the output file FMT_FCO2_PH_FIXED_QB0204.OUT is shown in **Figure 6.6.3**. The concentrations for both CO_2 (aq) and NaCl(halite) are bolded in the output listing and it can be seen that they are both zero as expected. The pH and f_{CO_2} have also been bolded, and a comparison of the output values with the input values does verify that the values of both remained unchanged as expected. Therefore, the acceptance criteria has been successfully met.

6.7 Test Case #7: Calculation of Chemical Invariant Points

6.7.1 Test Objectives

In this test case, FMT is used to calculate 3 chemical invariant points:

- 1) glaserite + shoenite + sylvite + halite
- 2) halite + teepelite + borax , and
- 3) $\text{KNaCO}_3 \cdot 6\text{H}_2\text{O} + \text{KCl} + \text{K}_2\text{CO}_3 \cdot \frac{3}{2}\text{H}_2\text{O}$.

It tests functional requirements R.1 and R.3.

6.7.2 Test Procedures

This test case was run using the script FMT_TEST_QB0204.COM. This command file is shown in **Figure 6.0.2**.

6.7.3 Input/Output Files

The following is a list of all files associated with Test Case #7:

Command file:

FMT_TEST_QB0204.COM

Input files:

FMT_INVAR_M.IN	(See Figure 6.7.1)
FMT_INVAR_M.INGUESS	(See Figure 6.7.2)
FMT_INVAR_B3.IN	(See Figure 6.7.3)
FMT_INVAR_B3.INGUESS	(See Figure 6.7.4)
FMT_INVAR_K4.IN	(See Figure 6.7.5)
FMT_INVAR_K4.INGUESS	(See Figure 6.7.6)

Output files:

FMT_INVAR_M_QB0204.OUT	(See Figure 6.7.7)
FMT_INVAR_B3_QB0204.OUT	(See Figure 6.7.8)
FMT_INVAR_K4_QB0204.OUT	(See Figure 6.7.9)

Figure 6.7.1 Listing of the Input File FMT_INVAR_M.IN

```
'Benchmark BATCH Problem: Invariant point M (Braitsch, 1971)'  
'CHEMFILE'  
'BATCH' 'UNUSED'  
'DISABLE SPECIES' 0  
'nSET_FCO2' 0.0  
'nSET_PH' 0.0  
  
'MOLES' 'EXACT'  
1.11120000E+02 Hydrogen  
5.55600000E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL
```

Figure 6.7.2 Listing of the Input File FMT_INVAR_M.INGUESS

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```
5.550868155779565E+01 H2O WATER 5.555999989948467E+01
1.000000000000000E-18 Na+ Na+ 0.000000000000000E+00
1.000000000000000E-18 K+ K+ 0.000000000000000E+00
0.000000000000000E+00 Ca++ Ca++ 0.000000000000000E+00
1.000000000000000E-18 Mg++ Mg++ 0.000000000000000E+00
1.000000000000000E-19 MgOH+ MgOH+ 0.000000000000000E+00
1.004224973864561E-07 H+ H+ 1.005153390085144E-07
1.000000000000000E-18 Cl- Cl- 0.000000000000000E+00
1.000000000000000E-18 SO4= SO4= 0.000000000000000E+00
1.000000000000000E-19 HSO4- HSO4- 0.000000000000000E+00
1.004224973864561E-07 OH- OH- 1.005153390085144E-07
0.000000000000000E+00 HCO3- HCO3- 0.000000000000000E+00
0.000000000000000E+00 CO3= CO3= 0.000000000000000E+00
0.000000000000000E+00 CO2 (aq) CO2 (aq) 0.000000000000000E+00
0.000000000000000E+00 CaCO3 (aq) CaCO3 (aq) 0.000000000000000E+00
0.000000000000000E+00 MgCO3 (aq) MgCO3 (aq) 0.000000000000000E+00
0.000000000000000E+00 B(OH) 3 (aq) B(OH) 3 (aq) 0.000000000000000E+00
0.000000000000000E+00 B(OH) 4- B(OH) 4- 0.000000000000000E+00
0.000000000000000E+00 B3O3 (OH) 4- B3O3 (OH) 4- 0.000000000000000E+00
0.000000000000000E+00 B4O5 (OH) 4= B4O5 (OH) 4= 0.000000000000000E+00
0.000000000000000E+00 CaB(OH) 4+ CaB(OH) 4+ 0.000000000000000E+00
0.000000000000000E+00 MgB(OH) 4+ MgB(OH) 4+ 0.000000000000000E+00
0.000000000000000E+00 Br- Br- 0.000000000000000E+00
0.000000000000000E+00 ClO4- perchlorate 0.000000000000000E+00
0.000000000000000E+00 NaOH(aq) to.titrate.base.only 0.000000000000000E+00
0.000000000000000E+00 HCl(aq) to.titrate.acid.only 0.000000000000000E+00
0.000000000000000E+00 HClO4(aq) to.titrate.acid.only 0.000000000000000E+00
0.000000000000000E+00 PosIon POSITIVE.ION 0.000000000000000E+00
0.000000000000000E+00 NegIon NEGATIVE.ION 0.000000000000000E+00
0.000000000000000E+00 PosIon(OH)(aq) to.titrate.base 0.000000000000000E+00
0.000000000000000E+00 HnegIon(aq) to.titrate.acid 0.000000000000000E+00
0.000000000000000E+00 H3PO4(aq) H3PO4(aq) 0.000000000000000E+00
0.000000000000000E+00 H2PO4- H2PO4- 0.000000000000000E+00
0.000000000000000E+00 HPO4= HPO4= 0.000000000000000E+00
0.000000000000000E+00 PO4=-- PO4=-- 0.000000000000000E+00
0.000000000000000E+00 Am+++ Am+++ 0.000000000000000E+00
0.000000000000000E+00 AmCO3+ AmCO3+ 0.000000000000000E+00
0.000000000000000E+00 Am(CO3) 2- Am(CO3) 2- 0.000000000000000E+00
0.000000000000000E+00 Am(CO3) 3-- Am(CO3) 3-- 0.000000000000000E+00
0.000000000000000E+00 AmOH++ (after_Cm(III)) 0.000000000000000E+00
0.000000000000000E+00 Am(OH) 2+ (after_Cm(III)) 0.000000000000000E+00
0.000000000000000E+00 Am(OH) 3(aq) (1e-9m_minimum) 0.000000000000000E+00
0.000000000000000E+00 Pu+++ Pu+++ 0.000000000000000E+00
0.000000000000000E+00 PuCO3+ PuCO3+ 0.000000000000000E+00
0.000000000000000E+00 Pu(CO3) 2- Pu(CO3) 2- 0.000000000000000E+00
0.000000000000000E+00 Pu(CO3) 3-- Pu(CO3) 3-- 0.000000000000000E+00
0.000000000000000E+00 PuOH++ (after_Cm(III)) 0.000000000000000E+00
0.000000000000000E+00 Pu(OH) 2+ (after_Cm(III)) 0.000000000000000E+00
0.000000000000000E+00 Pu(OH) 3(aq) (1e-9m_minimum) 0.000000000000000E+00
0.000000000000000E+00 Th++++ Th++++ 0.000000000000000E+00
0.000000000000000E+00 Th(CO3) 5=== Th(CO3) 5=== 0.000000000000000E+00
0.000000000000000E+00 Th(OH) 3(CO3)- Th(OH) 3(CO3)- 0.000000000000000E+00
0.000000000000000E+00 Th(OH) 4(aq) Th(OH) 4(aq) 0.000000000000000E+00
0.000000000000000E+00 Th(SO4) 2(aq) Th(SO4) 2(aq) 0.000000000000000E+00
0.000000000000000E+00 Th(SO4) 3= Th(SO4) 3= 0.000000000000000E+00
0.000000000000000E+00 U++++ U++++ 0.000000000000000E+00
0.000000000000000E+00 UOH+++ UOH+++ 0.000000000000000E+00
0.000000000000000E+00 U(CO3) 5=== U(CO3) 5=== 0.000000000000000E+00
0.000000000000000E+00 U(OH) 2(CO3) 2= U(OH) 2(CO3) 2= 0.000000000000000E+00
0.000000000000000E+00 U(OH) 4(CO3) 2== U(OH) 4(CO3) 2== 0.000000000000000E+00
0.000000000000000E+00 U(OH) 4(aq) U(OH) 4(aq) 0.000000000000000E+00
0.000000000000000E+00 U(SO4) 2(aq) U(SO4) 2(aq) 0.000000000000000E+00
0.000000000000000E+00 U(SO4) 3= U(SO4) 3= 0.000000000000000E+00
0.000000000000000E+00 NpO2+ NpO2+ 0.000000000000000E+00
0.000000000000000E+00 NpO2CO3- NpO2CO3- 0.000000000000000E+00
0.000000000000000E+00 NpO2(CO3) 2-- NpO2(CO3) 2-- 0.000000000000000E+00
0.000000000000000E+00 NpO2(CO3) 3=== NpO2(CO3) 3=== 0.000000000000000E+00
```

Figure 6.7.2 Listing of the Input File FMT_INVAR_M.INGUESS
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0.0000000000000000E+00	NpO2OH (aq)	NpO2OH (aq)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2 (OH) 2-	NpO2 (OH) 2-	0.0000000000000000E+00
0.0000000000000000E+00	HAc (aq)	AceticAcid	0.0000000000000000E+00
0.0000000000000000E+00	Ac-	Acetate-	0.0000000000000000E+00
0.0000000000000000E+00	H3Citrate (aq)	CitricAcid	0.0000000000000000E+00
0.0000000000000000E+00	H2Citrate-	H2Citrate-	0.0000000000000000E+00
0.0000000000000000E+00	HCitrate=	HCitrate=	0.0000000000000000E+00
0.0000000000000000E+00	Citrate=-	Citrate=-	0.0000000000000000E+00
0.0000000000000000E+00	H4EDTA (aq)	H4EDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	H3EDTA-	H3EDTA-	0.0000000000000000E+00
0.0000000000000000E+00	H2EDTA=	H2EDTA=	0.0000000000000000E+00
0.0000000000000000E+00	HEDTA=-	HEDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	EDTA=-	EDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	H2Ox (aq)	OxalicAcid	0.0000000000000000E+00
0.0000000000000000E+00	HOx-	Bioxalate-	0.0000000000000000E+00
0.0000000000000000E+00	Ox=	Oxalate=	0.0000000000000000E+00
0.0000000000000000E+00	HLactate (aq)	LacticAcid	0.0000000000000000E+00
0.0000000000000000E+00	Lactate-	Lactate-	0.0000000000000000E+00
0.0000000000000000E+00	AmAc++	AmAcetate++	0.0000000000000000E+00
0.0000000000000000E+00	AmCit (aq)	AmCitrate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	AmEDTA-	AmEDTA-	0.0000000000000000E+00
0.0000000000000000E+00	AmOx+	AmOxalate+	0.0000000000000000E+00
0.0000000000000000E+00	AmLac++	AmLactate++	0.0000000000000000E+00
0.0000000000000000E+00	PuAc++	PuAcetate++	0.0000000000000000E+00
0.0000000000000000E+00	PuCit (aq)	PuCitrate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	PuEDTA-	PuEDTA-	0.0000000000000000E+00
0.0000000000000000E+00	PuOx+	PuOxalate+	0.0000000000000000E+00
0.0000000000000000E+00	PuLac++	PuLactate++	0.0000000000000000E+00
0.0000000000000000E+00	ThAc+++	ThAc+++	0.0000000000000000E+00
0.0000000000000000E+00	ThCit+	ThCit+	0.0000000000000000E+00
0.0000000000000000E+00	ThEDTA (aq)	ThEDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	ThOx++	Th (C2O4) ++	0.0000000000000000E+00
0.0000000000000000E+00	ThLac+++	ThLac+++	0.0000000000000000E+00
0.0000000000000000E+00	UAc+++	U (IV) Ac+++	0.0000000000000000E+00
0.0000000000000000E+00	UCit+	U (IV) Cit+	0.0000000000000000E+00
0.0000000000000000E+00	UEDTA (aq)	U (IV) EDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	ULac+++	U (IV) Lac+++	0.0000000000000000E+00
0.0000000000000000E+00	UOx++	U (IV) Ox++	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Ac (aq)	NpO2Ac (aq)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Cit=	NpO2Citrate=	0.0000000000000000E+00
0.0000000000000000E+00	NpO2EDTA=-	NpO2EDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Ox-	NpO2Oxalate-	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Lac (aq)	NpO2Lactate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	MgAc+	MgAc+	0.0000000000000000E+00
0.0000000000000000E+00	MgCit-	MgCit-	0.0000000000000000E+00
0.0000000000000000E+00	MgEDTA=	MgEDTA=	0.0000000000000000E+00
0.0000000000000000E+00	MgOx (aq)	MgOx (aq)	0.0000000000000000E+00
0.0000000000000000E+00	MgLac+	MgLac+	0.0000000000000000E+00
0.0000000000000000E+00	CaAc+	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaCit-	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaEDTA=	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaOx (aq)	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaLac+	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	UnuCat#1+	UC#1+	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#1-	UA#1-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#2-	UA#2-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#3-	UA#3-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#4-	UA#4-	0.0000000000000000E+00
0.0000000000000000E+00	UnuNeu#1 (aq)	UN#1 (aq)	0.0000000000000000E+00
0.0000000000000000E+00	AmOHCO3 (c)	AmOHCO3 (c)	0.0000000000000000E+00
0.0000000000000000E+00	Am (OH) 3 (s)	Am (OH) 3 (s)	0.0000000000000000E+00
0.0000000000000000E+00	NaAm (CO3) 2.6H2O (c)		0.0000000000000000E+00
0.0000000000000000E+00	AmPO4 (c)	AmPO4 (c)	0.0000000000000000E+00
0.0000000000000000E+00	PuOHCO3 (c)	PuOHCO3 (c)	0.0000000000000000E+00
0.0000000000000000E+00	Pu (OH) 3 (s)	Pu (OH) 3 (s)	0.0000000000000000E+00
0.0000000000000000E+00	NaPu (CO3) 2.6H2O (c)		0.0000000000000000E+00
0.0000000000000000E+00	PuPO4 (c)	PuPO4 (c)	0.0000000000000000E+00

Figure 6.7.2 Listing of the Input File FMT_INVAR_M.INGUESS
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0.000000000000000E+00 ThO2(am) Hydrous_Thorium_Oxide 0.000000000000000E+00
0.000000000000000E+00 Th(SO4)2.9H2O(s) 0.000000000000000E+00
0.000000000000000E+00 Th(SO4)2.8H2O(s) 0.000000000000000E+00
0.000000000000000E+00 Th(SO4)2.Na2SO4.6H2O(16C,s) 0.000000000000000E+00
0.000000000000000E+00 Th(SO4)2.K2SO4.4H2O(16C,s) 0.000000000000000E+00
0.000000000000000E+00 Th(SO4)2.2K2SO4.2H2O(16C,s) 0.000000000000000E+00
0.000000000000000E+00 2[Th(SO4)2.7/2K2SO4(16C,s)] 0.000000000000000E+00
0.000000000000000E+00 UO2(am) Hydrous_U(IV)_Oxide 0.000000000000000E+00
0.000000000000000E+00 NpO2OH(aged) NpO2OH(aged) 0.000000000000000E+00
0.000000000000000E+00 NpO2OH(amor) NpO2OH(amor) 0.000000000000000E+00
0.000000000000000E+00 2[NaNpO2CO3.7/2H2O(s)] 0.000000000000000E+00
0.000000000000000E+00 Na3NpO2(CO3)2(s) Na3NpO2(CO3)2(s) 0.000000000000000E+00
0.000000000000000E+00 KNpO2CO3(s) KNpO2CO3(s) 0.000000000000000E+00
0.000000000000000E+00 K3NpO2(CO3)2(s) K3NpO2(CO3)2(s) 0.000000000000000E+00
0.000000000000000E+00 H2Ox.2H2O(s) H2C2O4.2H2O(s) 0.000000000000000E+00
0.000000000000000E+00 NaHOx.H2O(s) NaHC2O4.H2O(s) 0.000000000000000E+00
0.000000000000000E+00 Na2Ox(s) Na2C2O4(s) 0.000000000000000E+00
0.000000000000000E+00 CO2("solid",DISABLED) 0.000000000000000E+00
0.000000000000000E+00 CaSO4 Anhydrite 0.000000000000000E+00
8.000000000000000E+00 NaK3(SO4)2 Aphthalite/Glaserite 8.000000000000000E+00
0.000000000000000E+00 CaCl2.6H2O Antarcticite 0.000000000000000E+00
0.000000000000000E+00 CaCO3 Aragonite 0.000000000000000E+00
0.000000000000000E+00 K2SO4 Arcanite 0.000000000000000E+00
0.000000000000000E+00 MgCl2.6H2O Bischofite 0.000000000000000E+00
0.000000000000000E+00 Na2Mg(SO4)2.4H2O Bloedite 0.000000000000000E+00
0.000000000000000E+00 Mg(OH)2 Brucite 0.000000000000000E+00
0.000000000000000E+00 Na6CO3(SO4)2 Burkeite 0.000000000000000E+00
0.000000000000000E+00 CaCO3 Calcite 0.000000000000000E+00
0.000000000000000E+00 CaCl2.4H2O CaCl2 Tetrahydrate 0.000000000000000E+00
0.000000000000000E+00 Ca4Cl2(OH)6.13H2O CaOxychloride_A 0.000000000000000E+00
0.000000000000000E+00 Ca2C12(OH)2.H2O CaOxychloride_B 0.000000000000000E+00
0.000000000000000E+00 KMgCl3.6H2O Carnallite 0.000000000000000E+00
0.000000000000000E+00 MgSO4.7H2O Epsomite 0.000000000000000E+00
0.000000000000000E+00 CaNa2(CO3)2.5H2O Gaylussite 0.000000000000000E+00
0.000000000000000E+00 Na2Ca(SO4)2 Glauberite 0.000000000000000E+00
0.000000000000000E+00 CaSO4.2H2O Gypsum 0.000000000000000E+00
8.000000000000000E+00 NaCl Halite 8.000000000000000E+00
0.000000000000000E+00 MgSO4.6H2O Hexahydrate 0.000000000000000E+00
0.000000000000000E+00 KMgClSO4.3H2O Kainite 0.000000000000000E+00
0.000000000000000E+00 KHCO3 Kalicinite 0.000000000000000E+00
0.000000000000000E+00 MgSO4.H2O Kieserite 0.000000000000000E+00
0.000000000000000E+00 K2Mg(SO4)2.4H2O Leonite 0.000000000000000E+00
0.000000000000000E+00 Na4Ca(SO4)3.2H2O Labile_Salt 0.000000000000000E+00
0.000000000000000E+00 MgCO3 Magnesite 0.000000000000000E+00
0.000000000000000E+00 Mg2Cl(OH)3.4H2O MgOxychloride 0.000000000000000E+00
0.000000000000000E+00 KHSO4 Mercallite 0.000000000000000E+00
0.000000000000000E+00 Na2SO4.10H2O Mirabilite 0.000000000000000E+00
0.000000000000000E+00 K8H6(SO4)7 Misenite 0.000000000000000E+00
0.000000000000000E+00 NaHCO3 Nahcolite 0.000000000000000E+00
0.000000000000000E+00 Na2CO3.10H2O Natron 0.000000000000000E+00
0.000000000000000E+00 MgCO3.3H2O Nesquehonite 0.000000000000000E+00
8.000000000000000E+00 K2Mg(SO4)2.6H2O Picromerite/Schoen 8.000000000000000E+00
0.000000000000000E+00 Na2Ca(CO3)2.2H2O Pirssonite 0.000000000000000E+00
0.000000000000000E+00 K2MgCa2(SO4)4.2H2O Polyhalite 0.000000000000000E+00
0.000000000000000E+00 Ca(OH)2 Portlandite 0.000000000000000E+00
0.000000000000000E+00 K2CO3.3/2H2O Potassium Carbonate 0.000000000000000E+00
0.000000000000000E+00 K8H4(CO3)6.3H2O K-Sequicarbonate 0.000000000000000E+00
0.000000000000000E+00 KNaCO3.6H2O K-Na-Carbonate 0.000000000000000E+00
0.000000000000000E+00 K2NaH(CO3)2.2H2O Potassium Trona 0.000000000000000E+00
0.000000000000000E+00 K3H(SO4)2 Sesquipotassium Sulfate 0.000000000000000E+00
0.000000000000000E+00 Na3H(SO4)2 Sesquisodium Sulfate 0.000000000000000E+00
0.000000000000000E+00 Na2CO3.7H2O Na2CO3-Heptahydrate 0.000000000000000E+00
8.000000000000000E+00 KCl Sylvite 8.000000000000000E+00
0.000000000000000E+00 K2Ca(SO4)2.2H2O Syngenite 0.000000000000000E+00
0.000000000000000E+00 Mg2CaCl6.12H2O Tachyhydrite 0.000000000000000E+00
0.000000000000000E+00 Na2SO4 Thenardite 0.000000000000000E+00

Figure 6.7.2 Listing of the Input File FMT_INVAR_M.INGUESS
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```
0.000000000000000E+00 Na2CO3.H2O_____Thermonatrite 0.000000000000000E+00
0.000000000000000E+00 Na3H(CO3)2.2H2O_____Trona 0.000000000000000E+00
0.000000000000000E+00 Na2B4O7.10H2O_____Borax 0.000000000000000E+00
0.000000000000000E+00 B(OH)3_____Borix_Acid_Solid 0.000000000000000E+00
0.000000000000000E+00 KB5O8.4H2O_____K-Pentaborate_(30_C) 0.000000000000000E+00
0.000000000000000E+00 K2B4O7.4H2O_____K-Tetraborate_(30_C) 0.000000000000000E+00
0.000000000000000E+00 NaBO2.4H2O_____Sodium_Metaborate 0.000000000000000E+00
0.000000000000000E+00 NaB5O8.5H2O_____Sodium_Pentaborate 0.000000000000000E+00
0.000000000000000E+00 NaBO2.NaCl.2H2O_____Teepelite_(20_C) 0.000000000000000E+00
0.000000000000000E+00 CaMg(CO3)2_____Dolomite 0.000000000000000E+00
0.000000000000000E+00 Mg5(CO3)4(OH)2.4H2O_HydroMagne5424 0.000000000000000E+00
0.000000000000000E+00 Mg4(CO3)3(OH)2.3H2O_HydroMagne4323 0.000000000000000E+00
0.000000000000000E+00 H+(solid)_____to.set.aH+ 0.000000000000000E+00
0.000000000000000E+00 OH-/H2O(solid)_____to.set.aH+ 0.000000000000000E+00
```


Figure 6.7.3 Listing of the Input File FMT_INVAR_B3.IN

```
'Benchmark BATCH Problem: Invariant point B3'  
'CHEMFILE'  
'BATCH' 'UNUSED'  
'DISABLE SPECIES' 0  
'nSET_FC02' 0.0  
'nSET_PH' 0.0  
  
'MOLES' 'EXACT'  
1.11120000E+02 Hydrogen  
5.55600000E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL
```

Figure 6.7.4 Listing of the Input File FMT_INVAR_B3.INGUESS
(Page 1 of 4)

```
5.550868155779565E+01 H2O WATER 5.555999989948467E+01
1.000000000000000E-18 Na+ Na+ 0.000000000000000E+00
0.000000000000000E+00 K+ K+ 0.000000000000000E+00
0.000000000000000E+00 Ca++ Ca++ 0.000000000000000E+00
0.000000000000000E+00 Mg++ Mg++ 0.000000000000000E+00
0.000000000000000E+00 MgOH+ MgOH+ 0.000000000000000E+00
1.004224973864561E-07 H+ H+ 1.005153390085144E-07
1.000000000000000E-18 Cl- Cl- 0.000000000000000E+00
0.000000000000000E+00 SO4= SO4= 0.000000000000000E+00
0.000000000000000E+00 HSO4- HSO4- 0.000000000000000E+00
1.004224973864561E-07 OH- OH- 1.005153390085144E-07
0.000000000000000E+00 HCO3- HCO3- 0.000000000000000E+00
0.000000000000000E+00 CO3= CO3= 0.000000000000000E+00
0.000000000000000E+00 CO2 (aq) CO2 (aq) 0.000000000000000E+00
0.000000000000000E+00 CaCO3 (aq) CaCO3 (aq) 0.000000000000000E+00
0.000000000000000E+00 MgCO3 (aq) MgCO3 (aq) 0.000000000000000E+00
1.000000000000000E-18 B (OH) 3 (aq) B (OH) 3 (aq) 0.000000000000000E+00
0.000000000000000E+00 B (OH) 4- B (OH) 4- 0.000000000000000E+00
0.000000000000000E+00 B3O3 (OH) 4- B3O3 (OH) 4- 0.000000000000000E+00
0.000000000000000E+00 B4O5 (OH) 4= B4O5 (OH) 4= 0.000000000000000E+00
0.000000000000000E+00 CaB (OH) 4+ CaB (OH) 4+ 0.000000000000000E+00
0.000000000000000E+00 MgB (OH) 4+ MgB (OH) 4+ 0.000000000000000E+00
0.000000000000000E+00 Br- Br- 0.000000000000000E+00
0.000000000000000E+00 ClO4- perchlorate 0.000000000000000E+00
0.000000000000000E+00 NaOH (aq) to.titrate.base.only 0.000000000000000E+00
0.000000000000000E+00 HCl (aq) to.titrate.acid.only 0.000000000000000E+00
0.000000000000000E+00 HClO4 (aq) to.titrate.acid.only 0.000000000000000E+00
0.000000000000000E+00 PosIon POSITIVE.ION 0.000000000000000E+00
0.000000000000000E+00 NegIon NEGATIVE.ION 0.000000000000000E+00
0.000000000000000E+00 PosIon(OH) (aq) to.titrate.base 0.000000000000000E+00
0.000000000000000E+00 HNegIon (aq) to.titrate.acid 0.000000000000000E+00
0.000000000000000E+00 H3PO4 (aq) H3PO4 (aq) 0.000000000000000E+00
0.000000000000000E+00 H2PO4- H2PO4- 0.000000000000000E+00
0.000000000000000E+00 HPO4= HPO4= 0.000000000000000E+00
0.000000000000000E+00 PO4=- PO4=- 0.000000000000000E+00
0.000000000000000E+00 Am+++ Am+++ 0.000000000000000E+00
0.000000000000000E+00 AmCO3+ AmCO3+ 0.000000000000000E+00
0.000000000000000E+00 Am (CO3) 2- Am (CO3) 2- 0.000000000000000E+00
0.000000000000000E+00 Am (CO3) 3=- Am (CO3) 3=- 0.000000000000000E+00
0.000000000000000E+00 AmOH++ (after_Cm (III)) 0.000000000000000E+00
0.000000000000000E+00 Am (OH) 2+ (after_Cm (III)) 0.000000000000000E+00
0.000000000000000E+00 Am (OH) 3 (aq) (1e-9m_minimum) 0.000000000000000E+00
0.000000000000000E+00 Pu+++ Pu+++ 0.000000000000000E+00
0.000000000000000E+00 PuCO3+ PuCO3+ 0.000000000000000E+00
0.000000000000000E+00 Pu (CO3) 2- Pu (CO3) 2- 0.000000000000000E+00
0.000000000000000E+00 Pu (CO3) 3=- Pu (CO3) 3=- 0.000000000000000E+00
0.000000000000000E+00 PuOH++ (after_Cm (III)) 0.000000000000000E+00
0.000000000000000E+00 Pu (OH) 2+ (after_Cm (III)) 0.000000000000000E+00
0.000000000000000E+00 Pu (OH) 3 (aq) (1e-9m_minimum) 0.000000000000000E+00
0.000000000000000E+00 Th++++ Th++++ 0.000000000000000E+00
0.000000000000000E+00 Th (CO3) 5=== Th (CO3) 5=== 0.000000000000000E+00
0.000000000000000E+00 Th (OH) 3 (CO3) - Th (OH) 3 (CO3) - 0.000000000000000E+00
0.000000000000000E+00 Th (OH) 4 (aq) Th (OH) 4 (aq) 0.000000000000000E+00
0.000000000000000E+00 Th (SO4) 2 (aq) Th (SO4) 2 (aq) 0.000000000000000E+00
0.000000000000000E+00 Th (SO4) 3= Th (SO4) 3= 0.000000000000000E+00
0.000000000000000E+00 U++++ U++++ 0.000000000000000E+00
0.000000000000000E+00 UOH+++ UOH+++ 0.000000000000000E+00
0.000000000000000E+00 U (CO3) 5=== U (CO3) 5=== 0.000000000000000E+00
0.000000000000000E+00 U (OH) 2 (CO3) 2= U (OH) 2 (CO3) 2= 0.000000000000000E+00
0.000000000000000E+00 U (OH) 4 (CO3) 2== U (OH) 4 (CO3) 2== 0.000000000000000E+00
0.000000000000000E+00 U (OH) 4 (aq) U (OH) 4 (aq) 0.000000000000000E+00
0.000000000000000E+00 U (SO4) 2 (aq) U (SO4) 2 (aq) 0.000000000000000E+00
0.000000000000000E+00 U (SO4) 3= U (SO4) 3= 0.000000000000000E+00
0.000000000000000E+00 NpO2+ NpO2+ 0.000000000000000E+00
0.000000000000000E+00 NpO2CO3- NpO2CO3- 0.000000000000000E+00
0.000000000000000E+00 NpO2 (CO3) 2=- NpO2 (CO3) 2=- 0.000000000000000E+00
0.000000000000000E+00 NpO2 (CO3) 3=- NpO2 (CO3) 3=- 0.000000000000000E+00
```

Figure 6.7.4 Listing of the Input File FMT_INVAR_B3.INGUESS
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0.0000000000000000E+00	NpO2OH (aq)	NpO2OH (aq)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2 (OH) 2-	NpO2 (OH) 2-	0.0000000000000000E+00
0.0000000000000000E+00	HAc (aq)	AceticAcid	0.0000000000000000E+00
0.0000000000000000E+00	Ac-	Acetate-	0.0000000000000000E+00
0.0000000000000000E+00	H3Citrate (aq)	CitricAcid	0.0000000000000000E+00
0.0000000000000000E+00	H2Citrate-	H2Citrate-	0.0000000000000000E+00
0.0000000000000000E+00	HCitrate=	HCitrate=	0.0000000000000000E+00
0.0000000000000000E+00	Citrate=-	Citrate=-	0.0000000000000000E+00
0.0000000000000000E+00	H4EDTA (aq)	H4EDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	H3EDTA-	H3EDTA-	0.0000000000000000E+00
0.0000000000000000E+00	H2EDTA=	H2EDTA=	0.0000000000000000E+00
0.0000000000000000E+00	HEDTA=-	HEDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	EDTA=-	EDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	H2Ox (aq)	OxalicAcid	0.0000000000000000E+00
0.0000000000000000E+00	HOx-	Bioxalate-	0.0000000000000000E+00
0.0000000000000000E+00	Ox=	Oxalate=	0.0000000000000000E+00
0.0000000000000000E+00	HLactate (aq)	LacticAcid	0.0000000000000000E+00
0.0000000000000000E+00	Lactate-	Lactate-	0.0000000000000000E+00
0.0000000000000000E+00	AmAc++	AmAcetate++	0.0000000000000000E+00
0.0000000000000000E+00	AmCit (aq)	AmCitrate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	AmEDTA-	AmEDTA-	0.0000000000000000E+00
0.0000000000000000E+00	AmOx+	AmOxalate+	0.0000000000000000E+00
0.0000000000000000E+00	AmLac++	AmLactate++	0.0000000000000000E+00
0.0000000000000000E+00	PuAc++	PuAcetate++	0.0000000000000000E+00
0.0000000000000000E+00	PuCit (aq)	PuCitrate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	PuEDTA-	PuEDTA-	0.0000000000000000E+00
0.0000000000000000E+00	PuOx+	PuOxalate+	0.0000000000000000E+00
0.0000000000000000E+00	PuLac++	PuLactate++	0.0000000000000000E+00
0.0000000000000000E+00	ThAc+++	ThAc+++	0.0000000000000000E+00
0.0000000000000000E+00	ThCit+	ThCit+	0.0000000000000000E+00
0.0000000000000000E+00	ThEDTA (aq)	ThEDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	ThOx++	Th (C2O4) ++	0.0000000000000000E+00
0.0000000000000000E+00	ThLac+++	ThLac+++	0.0000000000000000E+00
0.0000000000000000E+00	UAc+++	U (IV) Ac+++	0.0000000000000000E+00
0.0000000000000000E+00	UCit+	U (IV) Cit+	0.0000000000000000E+00
0.0000000000000000E+00	UEDTA (aq)	U (IV) EDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	ULac+++	U (IV) Lac+++	0.0000000000000000E+00
0.0000000000000000E+00	UOx++	U (IV) Ox++	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Ac (aq)	NpO2Ac (aq)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Cit=	NpO2Citrate=	0.0000000000000000E+00
0.0000000000000000E+00	NpO2EDTA=-	NpO2EDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Ox-	NpO2Oxalate-	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Lac (aq)	NpO2Lactate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	MgAc+	MgAc+	0.0000000000000000E+00
0.0000000000000000E+00	MgCit-	MgCit-	0.0000000000000000E+00
0.0000000000000000E+00	MgEDTA=	MgEDTA=	0.0000000000000000E+00
0.0000000000000000E+00	MgOx (aq)	MgOx (aq)	0.0000000000000000E+00
0.0000000000000000E+00	MgLac+	MgLac+	0.0000000000000000E+00
0.0000000000000000E+00	CaAc+	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaCit-	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaEDTA=	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaOx (aq)	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaLac+	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	UnuCat#1+	UC#1+	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#1-	UA#1-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#2-	UA#2-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#3-	UA#3-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#4-	UA#4-	0.0000000000000000E+00
0.0000000000000000E+00	UnuNeu#1 (aq)	UN#1 (aq)	0.0000000000000000E+00
0.0000000000000000E+00	AmOHCO3 (c)	AmOHCO3 (c)	0.0000000000000000E+00
0.0000000000000000E+00	Am (OH) 3 (s)	Am (OH) 3 (s)	0.0000000000000000E+00
0.0000000000000000E+00	NaAm (CO3) 2.6H2O (c)		0.0000000000000000E+00
0.0000000000000000E+00	AmPO4 (c)	AmPO4 (c)	0.0000000000000000E+00
0.0000000000000000E+00	PuOHCO3 (c)	PuOHCO3 (c)	0.0000000000000000E+00
0.0000000000000000E+00	Pu (OH) 3 (s)	Pu (OH) 3 (s)	0.0000000000000000E+00
0.0000000000000000E+00	NaPu (CO3) 2.6H2O (c)		0.0000000000000000E+00
0.0000000000000000E+00	PuPO4 (c)	PuPO4 (c)	0.0000000000000000E+00

Figure 6.7.4 Listing of the Input File FMT_INVAR_B3.INGUESS
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0.0000000000000000E+00 ThO2(am)_____Hydrous_Thorium_Oxide 0.0000000000000000E+00
0.0000000000000000E+00 Th(SO4)2.9H2O(s)_____ 0.0000000000000000E+00
0.0000000000000000E+00 Th(SO4)2.8H2O(s)_____ 0.0000000000000000E+00
0.0000000000000000E+00 Th(SO4)2.Na2SO4.6H2O(16C,s)_____ 0.0000000000000000E+00
0.0000000000000000E+00 Th(SO4)2.K2SO4.4H2O(16C,s)_____ 0.0000000000000000E+00
0.0000000000000000E+00 Th(SO4)2.2K2SO4.2H2O(16C,s)_____ 0.0000000000000000E+00
0.0000000000000000E+00 2[Th(SO4)2.7/2K2SO4(16C,s)]_____ 0.0000000000000000E+00
0.0000000000000000E+00 UO2(am)_____Hydrous_U(IV)_Oxide 0.0000000000000000E+00
0.0000000000000000E+00 NpO2OH(aged)_____NpO2OH(aged) 0.0000000000000000E+00
0.0000000000000000E+00 NpO2OH(amor)_____NpO2OH(amor) 0.0000000000000000E+00
0.0000000000000000E+00 2[NaNpO2CO3.7/2H2O(s)]_____ 0.0000000000000000E+00
0.0000000000000000E+00 Na3NpO2(CO3)2(s)_____Na3NpO2(CO3)2(s) 0.0000000000000000E+00
0.0000000000000000E+00 KNpO2CO3(s)_____KNpO2CO3(s) 0.0000000000000000E+00
0.0000000000000000E+00 K3NpO2(CO3)2(s)_____K3NpO2(CO3)2(s) 0.0000000000000000E+00
0.0000000000000000E+00 H2Ox.2H2O(s)_____H2C2O4.2H2O(s) 0.0000000000000000E+00
0.0000000000000000E+00 NaHOx.H2O(s)_____NaHC2O4.H2O(s) 0.0000000000000000E+00
0.0000000000000000E+00 Na2Ox(s)_____Na2C2O4(s) 0.0000000000000000E+00
0.0000000000000000E+00 CO2("solid",DISABLED)_____ 0.0000000000000000E+00
0.0000000000000000E+00 CaSO4_____Anhydrite 0.0000000000000000E+00
0.0000000000000000E+00 NaK3(SO4)2_____Aphthitalite/Glaserite 0.0000000000000000E+00
0.0000000000000000E+00 CaCl2.6H2O_____Antarcticite 0.0000000000000000E+00
0.0000000000000000E+00 CaCO3_____Aragonite 0.0000000000000000E+00
0.0000000000000000E+00 K2SO4_____Arcanite 0.0000000000000000E+00
0.0000000000000000E+00 MgCl2.6H2O_____Bischofite 0.0000000000000000E+00
0.0000000000000000E+00 Na2Mg(SO4)2.4H2O_____Bloedite 0.0000000000000000E+00
0.0000000000000000E+00 Mg(OH)2_____Brucite 0.0000000000000000E+00
0.0000000000000000E+00 Na6CO3(SO4)2_____Burkeite 0.0000000000000000E+00
0.0000000000000000E+00 CaCO3_____Calcite 0.0000000000000000E+00
0.0000000000000000E+00 CaCl2.4H2O_____CaCl2 Tetrahydrate 0.0000000000000000E+00
0.0000000000000000E+00 Ca4Cl2(OH)6.13H2O_____CaOxychloride_A 0.0000000000000000E+00
0.0000000000000000E+00 Ca2Cl2(OH)2.H2O_____CaOxychloride_B 0.0000000000000000E+00
0.0000000000000000E+00 KMgCl3.6H2O_____Carnallite 0.0000000000000000E+00
0.0000000000000000E+00 MgSO4.7H2O_____Epsomite 0.0000000000000000E+00
0.0000000000000000E+00 CaNa2(CO3)2.5H2O_____Gaylussite 0.0000000000000000E+00
0.0000000000000000E+00 Na2Ca(SO4)2_____Glauberite 0.0000000000000000E+00
0.0000000000000000E+00 CaSO4.2H2O_____Gypsum 0.0000000000000000E+00
1.0000000000000000E+01 NaCl_____Halite 1.0000000000000000E+01
0.0000000000000000E+00 MgSO4.6H2O_____Hexahydrate 0.0000000000000000E+00
0.0000000000000000E+00 KMgClSO4.3H2O_____Kainite 0.0000000000000000E+00
0.0000000000000000E+00 KHCO3_____Kalicinite 0.0000000000000000E+00
0.0000000000000000E+00 MgSO4.H2O_____Kieserite 0.0000000000000000E+00
0.0000000000000000E+00 K2Mg(SO4)2.4H2O_____Leonite 0.0000000000000000E+00
0.0000000000000000E+00 Na4Ca(SO4)3.2H2O_____Labile_Salt 0.0000000000000000E+00
0.0000000000000000E+00 MgCO3_____Magnesite 0.0000000000000000E+00
0.0000000000000000E+00 Mg2Cl(OH)3.4H2O_____MgOxychloride 0.0000000000000000E+00
0.0000000000000000E+00 KHSO4_____Merallite 0.0000000000000000E+00
0.0000000000000000E+00 Na2SO4.10H2O_____Mirabilite 0.0000000000000000E+00
0.0000000000000000E+00 K8H6(SO4)7_____Misenite 0.0000000000000000E+00
0.0000000000000000E+00 NaHCO3_____Nahcolite 0.0000000000000000E+00
0.0000000000000000E+00 Na2CO3.10H2O_____Natron 0.0000000000000000E+00
0.0000000000000000E+00 MgCO3.3H2O_____Nesquehonite 0.0000000000000000E+00
0.0000000000000000E+00 K2Mg(SO4)2.6H2O_____Picromerite/Schoen 0.0000000000000000E+00
0.0000000000000000E+00 Na2Ca(CO3)2.2H2O_____Pirssonite 0.0000000000000000E+00
0.0000000000000000E+00 K2MgCa2(SO4)4.2H2O_____Polyhalite 0.0000000000000000E+00
0.0000000000000000E+00 Ca(OH)2_____Portlandite 0.0000000000000000E+00
0.0000000000000000E+00 K2CO3.3/2H2O_____Potassium Carbonate 0.0000000000000000E+00
0.0000000000000000E+00 K8H4(CO3)6.3H2O_____K-Sequicarbonate 0.0000000000000000E+00
0.0000000000000000E+00 KNaCO3.6H2O_____K-Na-Carbonate 0.0000000000000000E+00
0.0000000000000000E+00 K2NaH(CO3)2.2H2O_____Potassium Trona 0.0000000000000000E+00
0.0000000000000000E+00 K3H(SO4)2_____Sesquipotassium Sulfate 0.0000000000000000E+00
0.0000000000000000E+00 Na3H(SO4)2_____Sesquisodium Sulfate 0.0000000000000000E+00
0.0000000000000000E+00 Na2CO3.7H2O_____Na2CO3-Heptahydrate 0.0000000000000000E+00
0.0000000000000000E+00 KCl_____Sylvite 0.0000000000000000E+00
0.0000000000000000E+00 K2Ca(SO4)2.H2O_____Syngenite 0.0000000000000000E+00
0.0000000000000000E+00 Mg2CaCl6.12H2O_____Tachyhydrite 0.0000000000000000E+00
0.0000000000000000E+00 Na2SO4_____Thenardite 0.0000000000000000E+00
0.0000000000000000E+00 Na2CO3.H2O_____Thermonatrite 0.0000000000000000E+00

Figure 6.7.4 Listing of the Input File FMT_INVAR_B3.INGUESS
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```
0.0000000000000000E+00 Na3H(CO3)2.2H2O_____Trona 0.0000000000000000E+00
1.0000000000000000E+01 Na2B4O7.10H2O_____Borax 0.0000000000000000E+00
0.0000000000000000E+00 B(OH)3_____Borix_Acid_Solid 0.0000000000000000E+00
0.0000000000000000E+00 KB5O8.4H2O_____K-Pentaborate_(30_C) 0.0000000000000000E+00
0.0000000000000000E+00 K2B4O7.4H2O_____K-Tetraborate_(30_C) 0.0000000000000000E+00
0.0000000000000000E+00 NaBO2.4H2O_____Sodium_Metaborate 0.0000000000000000E+00
0.0000000000000000E+00 NaB5O8.5H2O_____Sodium_Pentaborate 0.0000000000000000E+00
1.0000000000000000E+01 NaBO2.NaCl.2H2O_____Teepelite_(20_C) 0.0000000000000000E+00
0.0000000000000000E+00 CaMg(CO3)2_____Dolomite 0.0000000000000000E+00
0.0000000000000000E+00 Mg5(CO3)4(OH)2.4H2O_HydroMagne5424 0.0000000000000000E+00
0.0000000000000000E+00 Mg4(CO3)3(OH)2.3H2O_HydroMagne4323 0.0000000000000000E+00
0.0000000000000000E+00 H+(solid)_____to.set.aH+ 0.0000000000000000E+00
0.0000000000000000E+00 OH-/H2O(solid)_____to.set.aH+ 0.0000000000000000E+00
```

Figure 6.7.5 Listing of the Input File FMT_INVAR_K4.IN

```
'Benchmark BATCH Problem: Invariant point K4'  
'CHEMFILE'  
'BATCH' 'UNUSED'  
'DISABLE_SPECIES' 0  
'nSET_FCO2' 0.0  
'nSET_PH' 0.0  
  
'MOLES' 'EXACT'  
1.11120000E+02 Hydrogen  
5.55600000E+01 Oxygen  
0.00000000E+00 Sodium  
0.00000000E+00 Potassium  
0.00000000E+00 Magnesium  
0.00000000E+00 Calcium  
0.00000000E+00 Chlorine  
0.00000000E+00 Sulfur  
0.00000000E+00 Carbon  
0.00000000E+00 PosIon:EL  
0.00000000E+00 NegIon:EL  
0.00000000E+00 Oxalate:EL  
0.00000000E+00 Boron  
0.00000000E+00 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
0.00000000E+00 Charge:EL
```


Figure 6.7.6 Listing of the Input File FMT_INVAR_K4.INGUESS
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5.550868155779565E+01	H2O	WATER	5.55599989948467E+01
1.000000000000000E-18	Na+	Na+	0.000000000000000E+00
1.000000000000000E-18	K+	K+	0.000000000000000E+00
0.000000000000000E+00	Ca++	Ca++	0.000000000000000E+00
0.000000000000000E+00	Mg++	Mg++	0.000000000000000E+00
0.000000000000000E+00	MgOH+	MgOH+	0.000000000000000E+00
1.004224973864561E-07	H+	H+	1.00515339085144E-07
1.000000000000000E-18	Cl-	Cl-	0.000000000000000E+00
0.000000000000000E+00	SO4=	SO4=	0.000000000000000E+00
0.000000000000000E+00	HSO4-	HSO4-	0.000000000000000E+00
1.004224973864561E-07	OH-	OH-	1.00515339085144E-07
1.000000000000000E-18	HCO3-	HCO3-	0.000000000000000E+00
0.000000000000000E+00	CO3=	CO3=	0.000000000000000E+00
0.000000000000000E+00	CO2 (aq)	CO2 (aq)	0.000000000000000E+00
0.000000000000000E+00	CaCO3 (aq)	CaCO3 (aq)	0.000000000000000E+00
0.000000000000000E+00	MgCO3 (aq)	MgCO3 (aq)	0.000000000000000E+00
0.000000000000000E+00	B(OH) 3 (aq)	B(OH) 3 (aq)	0.000000000000000E+00
0.000000000000000E+00	B(OH) 4-	B(OH) 4-	0.000000000000000E+00
0.000000000000000E+00	B3O3 (OH) 4-	B3O3 (OH) 4-	0.000000000000000E+00
0.000000000000000E+00	B4O5 (OH) 4=	B4O5 (OH) 4=	0.000000000000000E+00
0.000000000000000E+00	CaB(OH) 4+	CaB(OH) 4+	0.000000000000000E+00
0.000000000000000E+00	MgB(OH) 4+	MgB(OH) 4+	0.000000000000000E+00
0.000000000000000E+00	Br-	Br-	0.000000000000000E+00
0.000000000000000E+00	ClO4-	perchlorate	0.000000000000000E+00
0.000000000000000E+00	NaOH (aq)	to.titrate.base.only	0.000000000000000E+00
0.000000000000000E+00	HCl (aq)	to.titrate.acid.only	0.000000000000000E+00
0.000000000000000E+00	HClO4 (aq)	to.titrate.acid.only	0.000000000000000E+00
0.000000000000000E+00	PosIon	POSITIVE.ION	0.000000000000000E+00
0.000000000000000E+00	NegIon	NEGATIVE.ION	0.000000000000000E+00
0.000000000000000E+00	PosIon(OH) (aq)	to.titrate.base	0.000000000000000E+00
0.000000000000000E+00	HNegIon (aq)	to.titrate.acid	0.000000000000000E+00
0.000000000000000E+00	H3PO4 (aq)	H3PO4 (aq)	0.000000000000000E+00
0.000000000000000E+00	H2PO4-	H2PO4-	0.000000000000000E+00
0.000000000000000E+00	HPO4=	HPO4=	0.000000000000000E+00
0.000000000000000E+00	PO4=-	PO4=-	0.000000000000000E+00
0.000000000000000E+00	Am+++	Am+++	0.000000000000000E+00
0.000000000000000E+00	AmCO3+	AmCO3+	0.000000000000000E+00
0.000000000000000E+00	Am(CO3) 2-	Am(CO3) 2-	0.000000000000000E+00
0.000000000000000E+00	Am(CO3) 3=-	Am(CO3) 3=-	0.000000000000000E+00
0.000000000000000E+00	AmOH++	(after_Cm(III))	0.000000000000000E+00
0.000000000000000E+00	Am(OH) 2+	(after_Cm(III))	0.000000000000000E+00
0.000000000000000E+00	Am(OH) 3 (aq)	(1e-9m_minimum)	0.000000000000000E+00
0.000000000000000E+00	Pu+++	Pu+++	0.000000000000000E+00
0.000000000000000E+00	PuCO3+	PuCO3+	0.000000000000000E+00
0.000000000000000E+00	Pu(CO3) 2-	Pu(CO3) 2-	0.000000000000000E+00
0.000000000000000E+00	Pu(CO3) 3=-	Pu(CO3) 3=-	0.000000000000000E+00
0.000000000000000E+00	PuOH++	(after_Cm(III))	0.000000000000000E+00
0.000000000000000E+00	Pu(OH) 2+	(after_Cm(III))	0.000000000000000E+00
0.000000000000000E+00	Pu(OH) 3 (aq)	(1e-9m_minimum)	0.000000000000000E+00
0.000000000000000E+00	Th++++	Th++++	0.000000000000000E+00
0.000000000000000E+00	Th(CO3) 5===	Th(CO3) 5===	0.000000000000000E+00
0.000000000000000E+00	Th(OH) 3 (CO3) -	Th(OH) 3 (CO3) -	0.000000000000000E+00
0.000000000000000E+00	Th(OH) 4 (aq)	Th(OH) 4 (aq)	0.000000000000000E+00
0.000000000000000E+00	Th(SO4) 2 (aq)	Th(SO4) 2 (aq)	0.000000000000000E+00
0.000000000000000E+00	Th(SO4) 3=	Th(SO4) 3=	0.000000000000000E+00
0.000000000000000E+00	U++++	U++++	0.000000000000000E+00
0.000000000000000E+00	UOH+++	UOH+++	0.000000000000000E+00
0.000000000000000E+00	U(CO3) 5===	U(CO3) 5===	0.000000000000000E+00
0.000000000000000E+00	U(OH) 2 (CO3) 2=	U(OH) 2 (CO3) 2=	0.000000000000000E+00
0.000000000000000E+00	U(OH) 4 (CO3) 2==	U(OH) 4 (CO3) 2==	0.000000000000000E+00
0.000000000000000E+00	U(OH) 4 (aq)	U(OH) 4 (aq)	0.000000000000000E+00
0.000000000000000E+00	U(SO4) 2 (aq)	U(SO4) 2 (aq)	0.000000000000000E+00
0.000000000000000E+00	U(SO4) 3=	U(SO4) 3=	0.000000000000000E+00
0.000000000000000E+00	NpO2+	NpO2+	0.000000000000000E+00
0.000000000000000E+00	NpO2CO3-	NpO2CO3-	0.000000000000000E+00
0.000000000000000E+00	NpO2 (CO3) 2=-	NpO2 (CO3) 2=-	0.000000000000000E+00
0.000000000000000E+00	NpO2 (CO3) 3=-	NpO2 (CO3) 3=-	0.000000000000000E+00

Figure 6.7.6 Listing of the Input File FMT_INVAR_K4.INGUESS
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0.0000000000000000E+00	NpO2OH (aq)	NpO2OH (aq)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2 (OH) 2-	NpO2 (OH) 2-	0.0000000000000000E+00
0.0000000000000000E+00	HAc (aq)	AceticAcid	0.0000000000000000E+00
0.0000000000000000E+00	Ac-	Acetate-	0.0000000000000000E+00
0.0000000000000000E+00	H3Citrate (aq)	CitricAcid	0.0000000000000000E+00
0.0000000000000000E+00	H2Citrate-	H2Citrate-	0.0000000000000000E+00
0.0000000000000000E+00	HCitrate=	HCitrate=	0.0000000000000000E+00
0.0000000000000000E+00	Citrate=-	Citrate=-	0.0000000000000000E+00
0.0000000000000000E+00	H4EDTA (aq)	H4EDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	H3EDTA-	H3EDTA-	0.0000000000000000E+00
0.0000000000000000E+00	H2EDTA=	H2EDTA=	0.0000000000000000E+00
0.0000000000000000E+00	HEDTA=-	HEDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	EDTA==	EDTA==	0.0000000000000000E+00
0.0000000000000000E+00	H2Ox (aq)	OxalicAcid	0.0000000000000000E+00
0.0000000000000000E+00	HOx-	Bioxalate-	0.0000000000000000E+00
0.0000000000000000E+00	Ox=	Oxalate=	0.0000000000000000E+00
0.0000000000000000E+00	HLactate (aq)	LacticAcid	0.0000000000000000E+00
0.0000000000000000E+00	Lactate-	Lactate-	0.0000000000000000E+00
0.0000000000000000E+00	AmAc++	AmAcetate++	0.0000000000000000E+00
0.0000000000000000E+00	AmCit (aq)	AmCitrate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	AmEDTA-	AmEDTA-	0.0000000000000000E+00
0.0000000000000000E+00	AmOx+	AmOxalate+	0.0000000000000000E+00
0.0000000000000000E+00	AmLac++	AmLactate++	0.0000000000000000E+00
0.0000000000000000E+00	PuAc++	PuAcetate++	0.0000000000000000E+00
0.0000000000000000E+00	PuCit (aq)	PuCitrate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	PuEDTA-	PuEDTA-	0.0000000000000000E+00
0.0000000000000000E+00	PuOx+	PuOxalate+	0.0000000000000000E+00
0.0000000000000000E+00	PuLac++	PuLactate++	0.0000000000000000E+00
0.0000000000000000E+00	ThAc+++	ThAc+++	0.0000000000000000E+00
0.0000000000000000E+00	ThCit+	ThCit+	0.0000000000000000E+00
0.0000000000000000E+00	ThEDTA (aq)	ThEDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	ThOx++	Th (C2O4) ++	0.0000000000000000E+00
0.0000000000000000E+00	ThLac+++	ThLac+++	0.0000000000000000E+00
0.0000000000000000E+00	UAc+++	U (IV) Ac+++	0.0000000000000000E+00
0.0000000000000000E+00	UCit+	U (IV) Cit+	0.0000000000000000E+00
0.0000000000000000E+00	UEDTA (aq)	U (IV) EDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	ULac+++	U (IV) Lac+++	0.0000000000000000E+00
0.0000000000000000E+00	UOx++	U (IV) Ox++	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Ac (aq)	NpO2Ac (aq)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Cit=	NpO2Citrate=	0.0000000000000000E+00
0.0000000000000000E+00	NpO2EDTA=-	NpO2EDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Ox-	NpO2Oxalate-	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Lac (aq)	NpO2Lactate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	MgAc+	MgAc+	0.0000000000000000E+00
0.0000000000000000E+00	MgCit-	MgCit-	0.0000000000000000E+00
0.0000000000000000E+00	MgEDTA=	MgEDTA=	0.0000000000000000E+00
0.0000000000000000E+00	MgOx (aq)	MgOx (aq)	0.0000000000000000E+00
0.0000000000000000E+00	MgLac+	MgLac+	0.0000000000000000E+00
0.0000000000000000E+00	CaAc+	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaCit-	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaEDTA=	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaOx (aq)	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaLac+	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	UnuCat#1+	UC#1+	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#1-	UA#1-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#2-	UA#2-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#3-	UA#3-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#4-	UA#4-	0.0000000000000000E+00
0.0000000000000000E+00	UnuNeu#1 (aq)	UN#1 (aq)	0.0000000000000000E+00
0.0000000000000000E+00	AmOHCO3 (c)	AmOHCO3 (c)	0.0000000000000000E+00
0.0000000000000000E+00	Am (OH) 3 (s)	Am (OH) 3 (s)	0.0000000000000000E+00
0.0000000000000000E+00	NaAm (CO3) 2 . 6H2O (c)		0.0000000000000000E+00
0.0000000000000000E+00	AmPO4 (c)	AmPO4 (c)	0.0000000000000000E+00
0.0000000000000000E+00	PuOHCO3 (c)	PuOHCO3 (c)	0.0000000000000000E+00
0.0000000000000000E+00	Pu (OH) 3 (s)	Pu (OH) 3 (s)	0.0000000000000000E+00
0.0000000000000000E+00	NaPu (CO3) 2 . 6H2O (c)		0.0000000000000000E+00
0.0000000000000000E+00	PuPO4 (c)	PuPO4 (c)	0.0000000000000000E+00

Figure 6.7.6 Listing of the Input File FMT_INVAR_K4.INGUESS
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0.0000000000000000E+00	ThO2(am)_____Hydrous_Thorium_Oxide	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.9H2O(s)_____	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.8H2O(s)_____	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.Na2SO4.6H2O(l6C,s)_____	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.K2SO4.4H2O(l6C,s)_____	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.2K2SO4.2H2O(l6C,s)_____	0.0000000000000000E+00
0.0000000000000000E+00	2[Th(SO4)2.7/2K2SO4(l6C,s)]_____	0.0000000000000000E+00
0.0000000000000000E+00	UO2(am)_____Hydrous_U(IV)_Oxide	0.0000000000000000E+00
0.0000000000000000E+00	NpO2OH(aged)_____NpO2OH(aged)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2OH(amor)_____NpO2OH(amor)	0.0000000000000000E+00
0.0000000000000000E+00	2[NaNpO2CO3.7/2H2O(s)]_____	0.0000000000000000E+00
0.0000000000000000E+00	Na3NpO2(CO3)2(s)____Na3NpO2(CO3)2(s)	0.0000000000000000E+00
0.0000000000000000E+00	KNpO2CO3(s)_____KNpO2CO3(s)	0.0000000000000000E+00
0.0000000000000000E+00	K3NpO2(CO3)2(s)____K3NpO2(CO3)2(s)	0.0000000000000000E+00
0.0000000000000000E+00	H2Ox.2H2O(s)_____H2C2O4.2H2O(s)	0.0000000000000000E+00
0.0000000000000000E+00	NaHOx.H2O(s)_____NaHC2O4.H2O(s)	0.0000000000000000E+00
0.0000000000000000E+00	Na2Ox(s)_____Na2C2O4(s)	0.0000000000000000E+00
0.0000000000000000E+00	CO2("solid",DISABLED)_____	0.0000000000000000E+00
0.0000000000000000E+00	CaSO4_____Anhydrite	0.0000000000000000E+00
0.0000000000000000E+00	NaK3(SO4)2____Aphthitalite/Glaserite	0.0000000000000000E+00
0.0000000000000000E+00	CaCl2.6H2O_____Antarcticite	0.0000000000000000E+00
0.0000000000000000E+00	CaCO3_____Aragonite	0.0000000000000000E+00
0.0000000000000000E+00	K2SO4_____Arcanite	0.0000000000000000E+00
0.0000000000000000E+00	MgCl2.6H2O_____Bischofite	0.0000000000000000E+00
0.0000000000000000E+00	Na2Mg(SO4)2.4H2O_____Bloedite	0.0000000000000000E+00
0.0000000000000000E+00	Mg(OH)2_____Brucite	0.0000000000000000E+00
0.0000000000000000E+00	Na6CO3(SO4)2_____Burkeite	0.0000000000000000E+00
0.0000000000000000E+00	CaCO3_____Calcite	0.0000000000000000E+00
0.0000000000000000E+00	CaCl2.4H2O_____CaCl2_Tetrahydrate	0.0000000000000000E+00
0.0000000000000000E+00	Ca4Cl2(OH)6.13H2O____CaOxychloride_A	0.0000000000000000E+00
0.0000000000000000E+00	Ca2Cl2(OH)2.H2O____CaOxychloride_B	0.0000000000000000E+00
0.0000000000000000E+00	KMgCl3.6H2O_____Carnallite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.7H2O_____Epsomite	0.0000000000000000E+00
0.0000000000000000E+00	CaNa2(CO3)2.5H2O_____Gaylussite	0.0000000000000000E+00
0.0000000000000000E+00	Na2Ca(SO4)2_____Glauberite	0.0000000000000000E+00
0.0000000000000000E+00	CaSO4.2H2O_____Gypsum	0.0000000000000000E+00
0.0000000000000000E+00	NaCl_____Halite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.6H2O_____Hexahydrate	0.0000000000000000E+00
0.0000000000000000E+00	KMgClSO4.3H2O_____Kainite	0.0000000000000000E+00
0.0000000000000000E+00	KHCO3_____Kalicinite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.H2O_____Kieserite	0.0000000000000000E+00
0.0000000000000000E+00	K2Mg(SO4)2.4H2O_____Leonite	0.0000000000000000E+00
0.0000000000000000E+00	Na4Ca(SO4)3.2H2O_____Labile_Salt	0.0000000000000000E+00
0.0000000000000000E+00	MgCO3_____Magnesite	0.0000000000000000E+00
0.0000000000000000E+00	Mg2Cl(OH)3.4H2O_____MgOxychloride	0.0000000000000000E+00
0.0000000000000000E+00	KHSO4_____Mercurite	0.0000000000000000E+00
0.0000000000000000E+00	Na2SO4.10H2O_____Mirabilite	0.0000000000000000E+00
0.0000000000000000E+00	K8H6(SO4)7_____Misenite	0.0000000000000000E+00
0.0000000000000000E+00	NaHCO3_____Nahcolite	0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.10H2O_____Natron	0.0000000000000000E+00
0.0000000000000000E+00	MgCO3.3H2O_____Nesquehonite	0.0000000000000000E+00
0.0000000000000000E+00	K2Mg(SO4)2.6H2O_Picromerite/Schoen	0.0000000000000000E+00
0.0000000000000000E+00	Na2Ca(CO3)2.2H2O_____Pirssonite	0.0000000000000000E+00
0.0000000000000000E+00	K2MgCa2(SO4)4.2H2O_____Polyhalite	0.0000000000000000E+00
0.0000000000000000E+00	Ca(OH)2_____Portlandite	0.0000000000000000E+00
20.0000000000000000E+00	K2CO3.3/2H2O_____Potassium_Carbonate	0.0000000000000000E+00
0.0000000000000000E+00	K8H4(CO3)6.3H2O____K-SequiCarbonate	0.0000000000000000E+00
10.0000000000000000E+00	KNaCO3.6H2O_____K-Na-Carbonate	0.0000000000000000E+00
0.0000000000000000E+00	K2NaH(CO3)2.2H2O____Potassium_Trona	0.0000000000000000E+00
0.0000000000000000E+00	K3H(SO4)2____Sesquipotassium_Sulfate	0.0000000000000000E+00
0.0000000000000000E+00	Na3H(SO4)2____Sesquisodium_Sulfate	0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.7H2O_____Na2CO3-Heptahydrate	0.0000000000000000E+00
10.0000000000000000E+00	KCl_____Sylvite	0.0000000000000000E+00
0.0000000000000000E+00	K2Ca(SO4)2.H2O_____Syngenite	0.0000000000000000E+00
0.0000000000000000E+00	Mg2CaCl16.12H2O_____Tachyhydrite	0.0000000000000000E+00
0.0000000000000000E+00	Na2SO4_____Thenardite	0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.H2O_____Thermonatrite	0.0000000000000000E+00

Figure 6.7.6 Listing of the Input File FMT_INVAR_K4.INGUESS
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0.0000000000000000E+00	Na3H(CO3)2.2H2O	Trona	0.0000000000000000E+00
0.0000000000000000E+00	Na2B4O7.10H2O	Borax	0.0000000000000000E+00
0.0000000000000000E+00	B(OH)3	Borix Acid Solid	0.0000000000000000E+00
0.0000000000000000E+00	KB5O8.4H2O	K-Pentaborate_(30_C)	0.0000000000000000E+00
0.0000000000000000E+00	K2B4O7.4H2O	K-Tetraborate_(30_C)	0.0000000000000000E+00
0.0000000000000000E+00	NaBO2.4H2O	Sodium Metaborate	0.0000000000000000E+00
0.0000000000000000E+00	NaB5O8.5H2O	Sodium Pentaborate	0.0000000000000000E+00
0.0000000000000000E+00	NaBO2.NaCl.2H2O	Teepelite_(20_C)	0.0000000000000000E+00
0.0000000000000000E+00	CaMg(CO3)2	Dolomite	0.0000000000000000E+00
0.0000000000000000E+00	Mg5(CO3)4(OH)2.4H2O	HydroMagne5424	0.0000000000000000E+00
0.0000000000000000E+00	Mg4(CO3)3(OH)2.3H2O	HydroMagne4323	0.0000000000000000E+00
0.0000000000000000E+00	H+(solid)	to.set.aH+	0.0000000000000000E+00
0.0000000000000000E+00	OH-/H2O(solid)	to.set.aH+	0.0000000000000000E+00

Figure 6.7.7 Edited Listing of the Output File FMT_INVAR_M_QB0204.OUT

```

INPUT   file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_M.IN;1
INGUESS file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_M.INGUESS;1
OUTPUT  file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_M_QB0204.OUT;1
CHEMDAT file name is WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark BATCH Problem: Invariant point M (Braitsch, 1971)                FMT V2.4
FMT_ph_970407.chemdat
Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5=== by analogy
  
```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality
H2O	WATER	8.00789E-01
NaK3(SO4)2__Aphthitalite/Glaserite		7.87535E+00
Cl-	Cl-	6.72269E+00
K2Mg(SO4)2.6H2O_Picromerite/Schoen		4.19373E+00
KCl	Sylvite	3.78245E+00
Na+	Na+	2.62980E+00
MgOH+	MgOH+	4.60825E-06
Mg++	Mg++	2.04119E+00
NaCl	Halite	1.96470E+00
K+	K+	1.61358E+00
SO4=	SO4=	8.01529E-01
HSO4-	HSO4-	4.01186E-06
H+	H+	6.02997E-07
OH-	OH-	6.60712E-09

Figure 6.7.8 Listing of the Output File FMT_INVAR_B3_QB0204.OUT

```

INPUT   file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_B3.IN;1
INGUESS file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_B3.INGUESS;1
OUTPUT  file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_B3_QB0204.OUT;1
CHEMDAT file name is WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark BATCH Problem: Invariant point B3                FMT V2.4
FMT_ph_970407.chemdat
Added Th(CO3)5-Cl(-Na) Parm, assigned K+-Th(CO3)5=== by analogy
  
```

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

H2O	WATER	7.91610E-01
Na2B4O7.10H2O	Borax	9.95124E+00
NaBO2.NaCl.2H2O__Teepelite_(20_C)		8.49771E+00
Na+	Na+	7.31508E+00
Cl-	Cl-	5.80166E+00
NaCl	Halite	5.64304E+00
B(OH)4-	B(OH)4-	1.47092E+00
B4O5(OH)4=	B4O5(OH)4=	1.96498E-02
OH-	OH-	2.62592E-03
B(OH)3(aq)	B(OH)3(aq)	2.10038E-03
B3O3(OH)4-	B3O3(OH)4-	5.72800E-04
H+	H+	8.64686E-13

Figure 6.7.9 Listing of the Output File FMT_INVAR_K4_QB0204.OUT

INPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_K4.IN;1
INGUESS file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_K4.INGUESS;1
OUTPUT file name is:WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_INVAR_K4_QB0204.OUT;1
CHEMDAT file name is WP\$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark BATCH Problem: Invariant point K4 FMT V2.4
FMT_ph_970407.chemdat
Added Th(CO3)5-Cl(-Na) Parmas, assigned K+-Th(CO3)5=== by analogy

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name		Molality
H2O	WATER	6.86204E-01
K+	K+	1.50921E+01
CO3=	CO3=	8.29047E+00
KCl	Sylvite	6.10466E+00
KNaCO3.6H2O	K-Na-Carbonate	4.59926E+00
OH-	OH-	8.26824E-03
K2CO3.3/2H2O	Potassium Carbonate	6.13484E+00
Na+	Na+	1.74502E+00
Cl-	Cl-	2.39619E-01
HCO3-	HCO3-	8.26824E-03
CO2(aq)	CO2(aq)	8.53840E-12
H+	H+	6.52048E-14

6.7.4 Evaluation

The calculated total dissolved component concentrations for each chemical invariant point was to be compared with the experimental data from Braitsch (1971), Teeple (1929), and Linke (1958). The deviation of the model prediction from the experimental data was to be less than 30%.

Table 6.7.1 shows the experimental measurements from Braitsch(1971), **Table 6.7.2** shows the experimental data published by Teeple (1929), and **Table 6.7.3** shows the experimental measurements from Linke(1958).

For part 1, the calculated results from FMT are compared to the lab data published by Braitsch (1971). The calculated results from FMT for molality have been extracted from the FMT_INVAR_M_QB0204.OUT file and are shown in **Figure 6.7.7**. **Table 6.7.1** shows a summary of the comparison where

$$\text{difference} = \frac{m_{i,FMT}^{TTL} - m_{i,data}^{TTL}}{m_{i,data}^{TTL}} \times 100\% \quad (1)$$

The complete output files for each of these test cases have been retained in the SCMS.

Table 6.7.1 FMT Results versus Experimental Measurements from Braitsch (1971) for Invariant Problem M

	m_{Na}^{TTL}	m_k^{TTL}	m_{Mg}^{TTL}	m_{Cl}^{TTL}	m_{SO4}^{TTL}	Solid Phase
Braitsch	2.69	1.58	1.97	6.65	0.78	glaserite, shoenite
FMT	2.63	1.61	2.04	6.72	0.80	Sylvite, halite
Difference	-2.24%	2.13%	3.61%	1.09%	2.76%	

For part 2, the calculated results from FMT are compared to the lab data published by Teeple (1929). The calculated results from FMT for molality have been extracted from the FMT_INVAR_B3_QB0204.OUT file and are presented in **Figure 6.7.2**. A summary of the comparison can be found in **Table 6.7.2**.

Table 6.7.2 FMT Results versus Experimental Measurements from Teeple (1929) for Invariant Problem B2

	m_{Na}^{TTL}	m_{Cl}^{TTL}	m_{SO4}^{TTL}	m_{CO3}^{TTL}	m_B^{TTL}	Solid Phase
Teeple	6.97	5.68			1.37	halite,
FMT	7.32	5.80			1.55	teeplite
Difference	4.95%	2.14%			13.38%	borax

For part 3, the calculated results from FMT are compared to the lab data published by Linke(1958). The calculated results from FMT for molality have been extracted from the FMT_INVAR_K4_QB0204.OUT file and are presented in **Figure 6.7.9**. A summary of the comparison can be found in **Table 6.7.3**.

Table 6.7.3 FMT Results versus Experimental Measurements from Linke (1958) for Invariant Problem K4

	m_{Na}^{TTL}	m_k^{TTL}	m_{Cl}^{TTL}	m_{CO3}^{TTL}	Solid Phase
Linke	2.08	15.08	0.25	8.46	sylvite, KNaCO ₃ ·6H ₂ O, K ₂ CO ₃ ·3/2H ₂ O
FMT	1.75	15.09	0.24	8.30	
Difference	-16.10%	0.08%	-4.15%	-1.91%	

To be acceptable, the deviation of the model prediction from the experimental data was to be less than 30%. It can be seen that the deviations are well within this criteria. Therefore, the acceptance criteria is considered to have been met.

6.8 Test Case #8: Speciation of Am(III), Th(IV), and Np(V) in WIPP SPC Brine

6.8.1 Test Objectives

In this test case, FMT is used to calculate the speciation of Am(III), Th(IV), and Np(V) in WIPP SPC brine. This test case was to test if the chemical equilibrium calculation correctly for these radionuclides. It tests functional requirements R.2, R.3, and R.7.

6.8.2 Test Procedures

This test case was run using the script FMT_TEST_QB0204.COM. This command file is shown in **Figure 6.0.2**.

6.8.3 Input/Output Files

The following is a list of all files associated with Test Case #8:

Command file:

FMT_TEST_QB0204.COM

Input files:

FMT_AMTHNP_SPC.IN

(See **Figure 6.8.1**)

FMT_AMTHNP_SPC.INGUESS

(See **Figure 6.8.2**)

Output files:

FMT_AMTHNP_SPC_QB0204.OUT

(See **Figure 6.8.3**)

FMT_AMTHNP_SPC_QB0204.FOR088

(See **Figure 6.8.4**)

Figure 6.8.1 Listing of the Input File FMT_AMTHNP_SPC.IN

```
'Benchmark BATCH Problem: Am, Th, and Np speciation in SPC Brine'  
'CHEMFILE'  
'BATCH' 'UNUSED'  
'DISABLE_SPECIES' 0  
'nSET_FC02' 0.0  
'nSET_PH' 0.0  
  
'MOLES' 'EXACT'  
1.11084063E+02 Hydrogen  
5.57650233E+01 Oxygen  
2.00000000E+00 Sodium  
8.40000000E-01 Potassium  
1.55999951E+00 Magnesium  
1.64000000E-02 Calcium  
5.83000000E+00 Chlorine  
4.36000000E-02 Sulfur  
5.07101504E-03 Carbon  
0.00000000E+00 PosIon:EL  
5.32000000E-02 NegIon:EL  
0.00000000E+00 Oxalate:EL  
2.18000000E-02 Boron  
1.09000000E-02 Bromine  
0.00000000E+00 Acetate:EL  
0.00000000E+00 Th(IV)  
0.00000000E+00 Am(III)  
0.00000000E+00 U(VI)  
0.00000000E+00 Np(V)  
0.00000000E+00 ClO4:EL  
0.00000000E+00 Phosphorus  
0.00000000E+00 U(IV)  
0.00000000E+00 Lactate:EL  
0.00000000E+00 EDTA:EL  
0.00000000E+00 Citrate:EL  
0.00000000E+00 Electron:E  
2.71310752E-15 Charge:EL
```

Figure 6.8.2 Listing of the Input File FMT_AMTHNP_SPC.INGUESS
(Page 1 of 4)

5.550868155779565E+01	H2O	WATER	5.550852987299358E+01
2.000005465279027E+00	Na+	Na+	2.000000000000000E+00
8.400022954171912E-01	K+	K+	8.399999999999999E-01
1.638159739154425E-02	Ca++	Ca++	1.638155262666625E-02
1.553949485550957E+00	Mg++	Mg++	1.553945239178795E+00
1.781887387370465E-05	MgOH+	MgOH+	1.781882518127887E-05
1.023649977078501E-07	H+	H+	1.023647179819770E-07
5.830015931288362E+00	Cl-	Cl-	5.829999999999999E+00
4.360009709980041E-02	SO4=	SO4=	4.359997795677786E-02
2.204328234417293E-08	HSO4-	HSO4-	2.204322210799319E-08
8.807085749904686E-08	OH-	OH-	8.807061683379932E-08
1.403575296567849E-04	HCO3-	HCO3-	1.403571461113015E-04
1.589724448049007E-06	CO3=	CO3=	1.589720103917036E-06
2.184812806063298E-05	CO2 (aq)	CO2 (aq)	2.184806835773810E-05
1.186214775006496E-07	CaCO3 (aq)	CaCO3 (aq)	1.186211533517989E-07
1.243494380218998E-05	MgCO3 (aq)	MgCO3 (aq)	1.243490982206406E-05
2.025113540277278E-02	B(OH) 3 (aq)	B(OH) 3 (aq)	2.025108006387121E-02
3.623984586377640E-04	B(OH) 4-	B(OH) 4-	3.623974683361225E-04
1.247527254879187E-05	B3O3 (OH) 4-	B3O3 (OH) 4-	1.247523845846232E-05
3.543730901158883E-07	B4O5 (OH) 4=	B4O5 (OH) 4=	3.543721217446260E-07
1.832880226625685E-05	CaB(OH) 4+	CaB(OH) 4+	1.832875218038441E-05
1.129353597857759E-03	MgB(OH) 4+	MgB(OH) 4+	1.129350511749926E-03
1.090002978577070E-02	Br-	Br-	1.090000000000000E-02
0.000000000000000E+00	ClO4-	perchlorate	0.000000000000000E+00
0.000000000000000E+00	NaOH (aq)	to.titrate.base.only	0.000000000000000E+00
0.000000000000000E+00	HCl (aq)	to.titrate.acid.only	0.000000000000000E+00
0.000000000000000E+00	HClO4 (aq)	to.titrate.acid.only	0.000000000000000E+00
0.000000000000000E+00	PosIon	POSITIVE.ION	0.000000000000000E+00
5.320014537642213E-02	NegIon	NEGATIVE.ION	5.320000000000002E-02
0.000000000000000E+00	PosIon(OH) (aq)	to.titrate.base	0.000000000000000E+00
0.000000000000000E+00	HNegIon (aq)	to.titrate.acid	0.000000000000000E+00
0.000000000000000E+00	H3PO4 (aq)	H3PO4 (aq)	0.000000000000000E+00
0.000000000000000E+00	H2PO4-	H2PO4-	0.000000000000000E+00
0.000000000000000E+00	HPO4=	HPO4=	0.000000000000000E+00
0.000000000000000E+00	PO4--	PO4--	0.000000000000000E+00
1.000000000000000E-18	Am+++	Am+++	0.000000000000000E+00
0.000000000000000E+00	AmCO3+	AmCO3+	0.000000000000000E+00
0.000000000000000E+00	Am(CO3) 2-	Am(CO3) 2-	0.000000000000000E+00
0.000000000000000E+00	Am(CO3) 3--	Am(CO3) 3--	0.000000000000000E+00
0.000000000000000E+00	AmOH++	(after_Cm(III))	0.000000000000000E+00
0.000000000000000E+00	Am(OH) 2+	(after_Cm(III))	0.000000000000000E+00
0.000000000000000E+00	Am(OH) 3 (aq)	(1e-9m_minimum)	0.000000000000000E+00
0.000000000000000E+00	Pu+++	Pu+++	0.000000000000000E+00
0.000000000000000E+00	PuCO3+	PuCO3+	0.000000000000000E+00
0.000000000000000E+00	Pu(CO3) 2-	Pu(CO3) 2-	0.000000000000000E+00
0.000000000000000E+00	Pu(CO3) 3--	Pu(CO3) 3--	0.000000000000000E+00
0.000000000000000E+00	PuOH++	(after_Cm(III))	0.000000000000000E+00
0.000000000000000E+00	Pu(OH) 2+	(after_Cm(III))	0.000000000000000E+00
0.000000000000000E+00	Pu(OH) 3 (aq)	(1e-9m_minimum)	0.000000000000000E+00
1.000000000000000E-18	Th++++	Th++++	0.000000000000000E+00
0.000000000000000E+00	Th(CO3) 5===	Th(CO3) 5===	0.000000000000000E+00
0.000000000000000E+00	Th(OH) 3 (CO3) -	Th(OH) 3 (CO3) -	0.000000000000000E+00
0.000000000000000E+00	Th(OH) 4 (aq)	Th(OH) 4 (aq)	0.000000000000000E+00
0.000000000000000E+00	Th(SO4) 2 (aq)	Th(SO4) 2 (aq)	0.000000000000000E+00
0.000000000000000E+00	Th(SO4) 3=	Th(SO4) 3=	0.000000000000000E+00
0.000000000000000E+00	U++++	U++++	0.000000000000000E+00
0.000000000000000E+00	UOH+++	UOH+++	0.000000000000000E+00
0.000000000000000E+00	U(CO3) 5===	U(CO3) 5===	0.000000000000000E+00
0.000000000000000E+00	U(OH) 2 (CO3) 2=	U(OH) 2 (CO3) 2=	0.000000000000000E+00
0.000000000000000E+00	U(OH) 4 (CO3) 2==	U(OH) 4 (CO3) 2==	0.000000000000000E+00
0.000000000000000E+00	U(OH) 4 (aq)	U(OH) 4 (aq)	0.000000000000000E+00
0.000000000000000E+00	U(SO4) 2 (aq)	U(SO4) 2 (aq)	0.000000000000000E+00
0.000000000000000E+00	U(SO4) 3=	U(SO4) 3=	0.000000000000000E+00
1.000000000000000E-18	NpO2+	NpO2+	0.000000000000000E+00
0.000000000000000E+00	NpO2CO3-	NpO2CO3-	0.000000000000000E+00
0.000000000000000E+00	NpO2 (CO3) 2--	NpO2 (CO3) 2--	0.000000000000000E+00
0.000000000000000E+00	NpO2 (CO3) 3==	NpO2 (CO3) 3==	0.000000000000000E+00

Figure 6.8.2 Listing of the Input File FMT_AMTHNP_SPC.INGUESS
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0.0000000000000000E+00	NpO2OH (aq)	NpO2OH (aq)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2 (OH) 2-	NpO2 (OH) 2-	0.0000000000000000E+00
0.0000000000000000E+00	HAc (aq)	AceticAcid	0.0000000000000000E+00
0.0000000000000000E+00	Ac-	Acetate-	0.0000000000000000E+00
0.0000000000000000E+00	H3Citrate (aq)	CitricAcid	0.0000000000000000E+00
0.0000000000000000E+00	H2Citrate-	H2Citrate-	0.0000000000000000E+00
0.0000000000000000E+00	HCitrate=	HCitrate=	0.0000000000000000E+00
0.0000000000000000E+00	Citrate=-	Citrate=-	0.0000000000000000E+00
0.0000000000000000E+00	H4EDTA (aq)	H4EDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	H3EDTA-	H3EDTA-	0.0000000000000000E+00
0.0000000000000000E+00	H2EDTA=	H2EDTA=	0.0000000000000000E+00
0.0000000000000000E+00	HEDTA=-	HEDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	EDTA==	EDTA==	0.0000000000000000E+00
0.0000000000000000E+00	H2Ox (aq)	OxalicAcid	0.0000000000000000E+00
0.0000000000000000E+00	HOx-	Bioxalate-	0.0000000000000000E+00
0.0000000000000000E+00	Ox=	Oxalate=	0.0000000000000000E+00
0.0000000000000000E+00	HLactate (aq)	LacticAcid	0.0000000000000000E+00
0.0000000000000000E+00	Lactate-	Lactate-	0.0000000000000000E+00
0.0000000000000000E+00	AmAc++	AmAcetate++	0.0000000000000000E+00
0.0000000000000000E+00	AmCit (aq)	AmCitrate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	AmEDTA-	AmEDTA-	0.0000000000000000E+00
0.0000000000000000E+00	AmOx+	AmOxalate+	0.0000000000000000E+00
0.0000000000000000E+00	AmLac++	AmLactate++	0.0000000000000000E+00
0.0000000000000000E+00	PuAc++	PuAcetate++	0.0000000000000000E+00
0.0000000000000000E+00	PuCit (aq)	PuCitrate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	PuEDTA-	PuEDTA-	0.0000000000000000E+00
0.0000000000000000E+00	PuOx+	PuOxalate+	0.0000000000000000E+00
0.0000000000000000E+00	PuLac++	PuLactate++	0.0000000000000000E+00
0.0000000000000000E+00	ThAc+++	ThAc+++	0.0000000000000000E+00
0.0000000000000000E+00	ThCit+	ThCit+	0.0000000000000000E+00
0.0000000000000000E+00	ThEDTA (aq)	ThEDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	ThOx++	Th (C2O4) ++	0.0000000000000000E+00
0.0000000000000000E+00	ThLac+++	ThLac+++	0.0000000000000000E+00
0.0000000000000000E+00	UAc+++	U (IV) Ac+++	0.0000000000000000E+00
0.0000000000000000E+00	UCit+	U (IV) Cit+	0.0000000000000000E+00
0.0000000000000000E+00	UEDTA (aq)	U (IV) EDTA (aq)	0.0000000000000000E+00
0.0000000000000000E+00	ULac+++	U (IV) Lac+++	0.0000000000000000E+00
0.0000000000000000E+00	UOx++	U (IV) Ox++	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Ac (aq)	NpO2Ac (aq)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Cit=	NpO2Citrate=	0.0000000000000000E+00
0.0000000000000000E+00	NpO2EDTA=-	NpO2EDTA=-	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Ox-	NpO2Oxalate-	0.0000000000000000E+00
0.0000000000000000E+00	NpO2Lac (aq)	NpO2Lactate (aq)	0.0000000000000000E+00
0.0000000000000000E+00	MgAc+	MgAc+	0.0000000000000000E+00
0.0000000000000000E+00	MgCit-	MgCit-	0.0000000000000000E+00
0.0000000000000000E+00	MgEDTA=	MgEDTA=	0.0000000000000000E+00
0.0000000000000000E+00	MgOx (aq)	MgOx (aq)	0.0000000000000000E+00
0.0000000000000000E+00	MgLac+	MgLac+	0.0000000000000000E+00
0.0000000000000000E+00	CaAc+	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaCit-	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaEDTA=	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaOx (aq)	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	CaLac+	(Mg-analog)	0.0000000000000000E+00
0.0000000000000000E+00	UnuCat#1+	UC#1+	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#1-	UA#1-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#2-	UA#2-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#3-	UA#3-	0.0000000000000000E+00
0.0000000000000000E+00	UnuAn#4-	UA#4-	0.0000000000000000E+00
0.0000000000000000E+00	UnuNeu#1 (aq)	UN#1 (aq)	0.0000000000000000E+00
0.0000000000000000E+00	AmOHCO3 (c)	AmOHCO3 (c)	0.0000000000000000E+00
1.0000000000000000E-05	Am (OH) 3 (s)	Am (OH) 3 (s)	0.0000000000000000E+00
0.0000000000000000E+00	NaAm (CO3) 2.6H2O (c)		0.0000000000000000E+00
0.0000000000000000E+00	AmPO4 (c)	AmPO4 (c)	0.0000000000000000E+00
0.0000000000000000E+00	PuOHCO3 (c)	PuOHCO3 (c)	0.0000000000000000E+00
0.0000000000000000E+00	Pu (OH) 3 (s)	Pu (OH) 3 (s)	0.0000000000000000E+00
0.0000000000000000E+00	NaPu (CO3) 2.6H2O (c)		0.0000000000000000E+00
0.0000000000000000E+00	PuPO4 (c)	PuPO4 (c)	0.0000000000000000E+00

Figure 6.8.2 Listing of the Input File FMT_AMTHNP_SPC.INGUESS
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1.0000000000000000E-05	ThO2(am)_____Hydrous_Thorium_Oxide	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.9H2O(s)_____	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.8H2O(s)_____	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.Na2SO4.6H2O(16C,s)_____	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.K2SO4.4H2O(16C,s)_____	0.0000000000000000E+00
0.0000000000000000E+00	Th(SO4)2.2K2SO4.2H2O(16C,s)_____	0.0000000000000000E+00
0.0000000000000000E+00	2[Th(SO4)2.7/2K2SO4(16C,s)]_____	0.0000000000000000E+00
0.0000000000000000E+00	UO2(am)_____Hydrous_U(IV)_Oxide	0.0000000000000000E+00
1.0000000000000000E-05	NpO2OH(aged)_____NpO2OH(aged)	0.0000000000000000E+00
0.0000000000000000E+00	NpO2OH(amor)_____NpO2OH(amor)	0.0000000000000000E+00
0.0000000000000000E+00	2[NaNpO2CO3.7/2H2O(s)]_____	0.0000000000000000E+00
0.0000000000000000E+00	Na3NpO2(CO3)2(s)____Na3NpO2(CO3)2(s)	0.0000000000000000E+00
0.0000000000000000E+00	KNpO2CO3(s)_____KNpO2CO3(s)	0.0000000000000000E+00
0.0000000000000000E+00	K3NpO2(CO3)2(s)____K3NpO2(CO3)2(s)	0.0000000000000000E+00
0.0000000000000000E+00	H2Ox.2H2O(s)_____H2C2O4.2H2O(s)	0.0000000000000000E+00
0.0000000000000000E+00	NaHOx.H2O(s)_____NaHC2O4.H2O(s)	0.0000000000000000E+00
0.0000000000000000E+00	Na2Ox(s)_____Na2C2O4(s)	0.0000000000000000E+00
0.0000000000000000E+00	CO2("solid",DISABLED)_____	0.0000000000000000E+00
0.0000000000000000E+00	CaSO4_____Anhydrite	0.0000000000000000E+00
0.0000000000000000E+00	NaK3(SO4)2____Aphthitalite/Glaserite	0.0000000000000000E+00
0.0000000000000000E+00	CaCl2.6H2O_____Antarcticite	0.0000000000000000E+00
0.0000000000000000E+00	CaCO3_____Aragonite	0.0000000000000000E+00
0.0000000000000000E+00	K2SO4_____Arcanite	0.0000000000000000E+00
0.0000000000000000E+00	MgCl2.6H2O_____Bischofite	0.0000000000000000E+00
0.0000000000000000E+00	Na2Mg(SO4)2.4H2O_____Bloeditite	0.0000000000000000E+00
0.0000000000000000E+00	Mg(OH)2_____Brucite	0.0000000000000000E+00
0.0000000000000000E+00	Na6CO3(SO4)2_____Burkeite	0.0000000000000000E+00
0.0000000000000000E+00	CaCO3_____Calcite	0.0000000000000000E+00
0.0000000000000000E+00	CaCl2.4H2O_____CaCl2_Tetrahydrate	0.0000000000000000E+00
0.0000000000000000E+00	Ca4Cl2(OH)6.13H2O____CaOxychloride_A	0.0000000000000000E+00
0.0000000000000000E+00	Ca2Cl2(OH)2.H2O____CaOxychloride_B	0.0000000000000000E+00
0.0000000000000000E+00	KMgCl3.6H2O_____Carnallite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.7H2O_____Epsomite	0.0000000000000000E+00
0.0000000000000000E+00	CaNa2(CO3)2.5H2O_____Gaylussite	0.0000000000000000E+00
0.0000000000000000E+00	Na2Ca(SO4)2_____Glauberite	0.0000000000000000E+00
0.0000000000000000E+00	CaSO4.2H2O_____Gypsum	0.0000000000000000E+00
0.0000000000000000E+00	NaCl_____Halite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.6H2O_____Hexahydrate	0.0000000000000000E+00
0.0000000000000000E+00	KMgClSO4.3H2O_____Kainite	0.0000000000000000E+00
0.0000000000000000E+00	KHCO3_____Kalicinite	0.0000000000000000E+00
0.0000000000000000E+00	MgSO4.H2O_____Kieserite	0.0000000000000000E+00
0.0000000000000000E+00	K2Mg(SO4)2.4H2O_____Leonite	0.0000000000000000E+00
0.0000000000000000E+00	Na4Ca(SO4)3.2H2O_____Labile_Salt	0.0000000000000000E+00
4.894679949810916E-03	MgCO3_____Magnesite	4.894666574451630E-03
0.0000000000000000E+00	Mg2Cl(OH)3.4H2O_____MgOxychloride	0.0000000000000000E+00
0.0000000000000000E+00	KHSO4_____Mercallite	0.0000000000000000E+00
0.0000000000000000E+00	Na2SO4.10H2O_____Mirabilite	0.0000000000000000E+00
0.0000000000000000E+00	K8H6(SO4)7_____Misenite	0.0000000000000000E+00
0.0000000000000000E+00	NaHCO3_____Nahcolite	0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.10H2O_____Natron	0.0000000000000000E+00
0.0000000000000000E+00	MgCO3.3H2O_____Nesquehonite	0.0000000000000000E+00
0.0000000000000000E+00	K2Mg(SO4)2.6H2O_Picromerite/Schoen	0.0000000000000000E+00
0.0000000000000000E+00	Na2Ca(CO3)2.2H2O_____Pirssonite	0.0000000000000000E+00
0.0000000000000000E+00	K2MgCa2(SO4)4.2H2O_____Polyhalite	0.0000000000000000E+00
0.0000000000000000E+00	Ca(OH)2_____Portlandite	0.0000000000000000E+00
0.0000000000000000E+00	K2CO3.3/2H2O____Potassium_Carbonate	0.0000000000000000E+00
0.0000000000000000E+00	K8H4(CO3)6.3H2O____K-Sequicarbonate	0.0000000000000000E+00
0.0000000000000000E+00	KNaCO3.6H2O_____K-Na-Carbonate	0.0000000000000000E+00
0.0000000000000000E+00	K2NaH(CO3)2.2H2O____Potassium_Trona	0.0000000000000000E+00
0.0000000000000000E+00	K3H(SO4)2____Sesquipotassium_Sulfate	0.0000000000000000E+00
0.0000000000000000E+00	Na3H(SO4)2____Sesquisodium_Sulfate	0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.7H2O____Na2CO3-Heptahydrate	0.0000000000000000E+00
0.0000000000000000E+00	KCl_____Sylvite	0.0000000000000000E+00
0.0000000000000000E+00	K2Ca(SO4)2.H2O_____Syngenite	0.0000000000000000E+00
0.0000000000000000E+00	Mg2CaCl6.12H2O_____Tachyhydrite	0.0000000000000000E+00
0.0000000000000000E+00	Na2SO4_____Thenardite	0.0000000000000000E+00
0.0000000000000000E+00	Na2CO3.H2O_____Thermonatrite	0.0000000000000000E+00

Figure 6.8.2 Listing of the Input File FMT_AMTHNP_SPC.INGUESS
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```
0.0000000000000000E+00 Na3H(CO3)2.2H2O_____Trona 0.0000000000000000E+00
0.0000000000000000E+00 Na2B4O7.10H2O_____Borax 0.0000000000000000E+00
0.0000000000000000E+00 B(OH)3_____Borix_Acid_Solid 0.0000000000000000E+00
0.0000000000000000E+00 KB5O8.4H2O_____K-Pentaborate_(30_C) 0.0000000000000000E+00
0.0000000000000000E+00 K2B4O7.4H2O_____K-Tetraborate_(30_C) 0.0000000000000000E+00
0.0000000000000000E+00 NaBO2.4H2O_____Sodium_Metaborate 0.0000000000000000E+00
0.0000000000000000E+00 NaB5O8.5H2O_____Sodium_Pentaborate 0.0000000000000000E+00
0.0000000000000000E+00 NaBO2.NaCl.2H2O_____Teepelite_(20_C) 0.0000000000000000E+00
0.0000000000000000E+00 CaMg(CO3)2_____Dolomite 0.0000000000000000E+00
0.0000000000000000E+00 Mg5(CO3)4(OH)2.4H2O_HydroMagne5424 0.0000000000000000E+00
0.0000000000000000E+00 Mg4(CO3)3(OH)2.3H2O_HydroMagne4323 0.0000000000000000E+00
0.0000000000000000E+00 H+(solid)_____to.set.aH+ 0.0000000000000000E+00
0.0000000000000000E+00 OH-/H2O(solid)_____to.set.aH+ 0.0000000000000000E+00
```

Figure 6.8.3 Edited Listing of the Output File FMT_AMTHNP_SPC_QB0204.OUT
 (Page 1 of 2)

```

INPUT   file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMTHNP_SPC.IN;1
INGUESS file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMTHNP_SPC.INGUESS;1
OUTPUT  file name is:WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_AMTHNP_SPC_QB0204.OUT;1
CHEMDAT file name is WP$NONPA_TESTROOT:[000000.FMT.TESTCASES]FMT_PH_970407.CHEMDAT;1
Temperature is Hard Coded as 298.15K
Benchmark BATCH Problem: Am, Th, and Np speciation in SPC Brine           FMT V2.4
FMT_PH_970407.chemdat
Added Th(CO3)5-Cl(-Na) ParmS, assigned K+-Th(CO3)5=== by analogy
  
```

Species Name	Phase	Std Chemical Potential, u/RT
3 K+	K+ aqueous	-113.9570
9 SO4=	SO4= aqueous	-300.3860
11 OH-	OH- aqueous	-63.4350
13 CO3=	CO3= aqueous	-212.9440
36 Am+++	Am+++ aqueous	-241.6940
37 AmCO3+	AmCO3+ aqueous	-472.0600
38 Am(CO3)2-	Am(CO3)2- aqueous	-695.8800
39 Am(CO3)3=-	Am(CO3)3=- aqueous	-915.4600
40 AmOH++	(after_Cm(III)) aqueous	-315.3520
41 Am(OH)2+	(after_Cm(III)) aqueous	-392.2810
42 Am(OH)3(aq)	(1e-9m_minimum) aqueous	-471.6030
50 Th++++	Th++++ aqueous	-284.2270
51 Th(CO3)5===	Th(CO3)5=== aqueous	-1411.3780
52 Th(OH)3(CO3)-	Th(OH)3(CO3)- aqueous	-775.6270
53 Th(OH)4(aq)	Th(OH)4(aq) aqueous	-622.8400
54 Th(SO4)2(aq)	Th(SO4)2(aq) aqueous	-911.6900
55 Th(SO4)3=	Th(SO4)3= aqueous	-1214.0000
64 NpO2+	NpO2+ aqueous	-369.1090
65 NpO2CO3-	NpO2CO3- aqueous	-593.6350
66 NpO2(CO3)2=-	NpO2(CO3)2=- aqueous	-809.8950
67 NpO2(CO3)3=-	NpO2(CO3)3=- aqueous	-1020.3060
68 NpO2OH(aq)	NpO2OH(aq) aqueous	-438.7380
69 NpO2(OH)2-	NpO2(OH)2- aqueous	-506.2490
127 AmOHCO3(c)	AmOHCO3(c) solid	-569.9800
147 KNpO2CO3(s)	KNpO2CO3(s) solid	-727.3300

```

# inversions for batch pblm           68
1Benchmark BATCH Problem: Am, Th, and Np speciation in SPC Brine           FMT V2.4
FMT_PH_970407.chemdat
Added Th(CO3)5-Cl(-Na) ParmS, assigned K+-Th(CO3)5=== by analogy
  Pressure= 1.00000E+00 [=] ATM      Temperature= 2.98E+02 [=] Kelvin
  
```

Elemental Abundances for Flash Problem

Total Moles	Aq. Molality	Aq. Molarity	Aq. mg/liter
-------------	--------------	--------------	--------------

TABLE OF CONCENTRATIONS FOR BATCH SYSTEM

Species Name	Activity	Total Moles
H2O	WATER	7.58695E-01
K+	K+	5.55087E+01
NegIon	NEGATIVE.ION	2.90955E-01
SO4=	SO4=	8.39998E-01
B(OH)3(aq)	B(OH)3(aq)	5.32002E-02
MgCO3	Magnesite	1.44317E-03
MgB(OH)4+	MgB(OH)4+	4.36001E-02
Th(CO3)5===	Th(CO3)5===	3.14525E-02
NpO2+	NpO2+	2.01870E-02
AmOHCO3(c)	AmOHCO3(c)	1.00000E+00
B(OH)4-	B(OH)4-	4.84220E-03
HCO3-	HCO3-	1.72388E-03
CO2(aq)	CO2(aq)	1.76256E-29
MgOH+	MgOH+	1.7623E-03
		9.98187E-06
		6.00263E-06
		6.21811E-06
		3.77471E-04
		1.34347E-04
		2.00138E-05
		1.86180E-05

Figure 6.8.3 Edited Listing of the Output File FMT_AMTHNP_SPC_QB0204.OUT
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B3O3 (OH) 4-	B3O3 (OH) 4-	5.36232E-06	1.29116E-05
MgCO3 (aq)	MgCO3 (aq)	1.24349E-05	1.24349E-05
Am+++	Am+++	1.14190E-07	3.56989E-06
CO3=	CO3=	9.81505E-09	1.58986E-06
B4O5 (OH) 4=	B4O5 (OH) 4=	1.84032E-09	3.82003E-07
NpO2CO3-	NpO2CO3-	9.20596E-09	1.36971E-07
AmCO3+	AmCO3+	4.12856E-08	1.81972E-07
CaCO3 (aq)	CaCO3 (aq)	1.18615E-07	1.18615E-07
H+	H+	2.99124E-07	9.79727E-08
OH-	OH-	2.55597E-08	9.20254E-08
HSO4-	HSO4-	4.10975E-08	2.10976E-08
AmOH++	(after_Cm(III))	8.03482E-11	1.87358E-08
Th(OH)3(CO3)-	Th(OH)3(CO3)-	4.69134E-09	1.76010E-08
Am(OH)2+	(after_Cm(III))	1.48903E-12	1.11489E-08
NpO2OH(aq)	NpO2OH(aq)	1.09586E-10	1.00437E-09
Th(OH)4(aq)	Th(OH)4(aq)	4.60620E-10	4.60620E-10
NpO2(CO3)2=-	NpO2(CO3)2=-	2.48933E-15	1.95611E-10
Am(CO3)2-	Am(CO3)2-	2.14327E-11	8.04118E-11
Am(CO3)3=-	Am(CO3)3=-	1.60306E-16	6.25941E-11
Th(SO4)3=	Th(SO4)3=	1.19821E-12	6.16159E-11
NpO2(CO3)3=-	NpO2(CO3)3=-	1.94047E-24	3.33920E-12
Th(SO4)2(aq)	Th(SO4)2(aq)	1.21236E-10	4.12197E-12
Am(OH)3(aq)	(1e-9m_minimum)	3.02061E-13	3.02061E-13
NpO2(OH)2-	NpO2(OH)2-	1.65004E-16	1.01641E-14
Th++++	Th++++	1.49019E-16	6.50005E-15
KNpO2CO3(s)	KNpO2CO3(s)	1.00000E+00	3.85920E-06

6.8.4 Evaluation

The acceptance criteria for this test case was that mass balance and equilibrium constraints on Am(III), Th(IV), and Np(V) are satisfied. They will be checked by hand calculations.

All problems solved with FMT should satisfy mass balance and equilibrium constraints. All chemical species should satisfy mass balance and equilibrium constraints. For example, for the general balanced chemical reaction

$$\sum_i r_i R_i = \sum_j p_j P_j$$

where r_i = stoichiometric coefficients of the reactant species R_i
 p_j = stoichiometric coefficients of the product species P_j

Equilibrium is given by:

$$\frac{\prod_j a_j^{p_j}}{\prod_i a_i^{r_i}} = \text{EXP} \left(-\sum_j p_j \frac{\mu_j^0}{RT} + \sum_i r_i \frac{\mu_i^0}{RT} \right)$$

where $\frac{\mu_i^0}{RT}$ and $\frac{\mu_j^0}{RT}$ are taken from the CHEMDAT file
 a_i and a_j are the calculated activities for species R_i and P_j respectively

Mass balance is given by:

$$\sum_j \nu_{ij} M_j = A_i \quad i = 1, 2, \dots, I$$

where ν_{ij} = the stoichiometric coefficient of element i in species j
 M_j = "Total Moles" of species j
 A_i = "Elemental Abundance Total Moles" for element i

Mass Balances

The mass balance equations are written disregarding charge on the chemical species.
(M = total number of moles of given species or element.)

Mass Balance for Americium

Total moles of elemental americium =

$$\begin{aligned} & M(\text{AmOHCO}_3) + M(\text{Am}) + M(\text{AmCO}_3) + M(\text{AmOH}) + M(\text{Am}(\text{OH})_2) + M(\text{Am}(\text{CO}_3)_2) + M(\text{Am}(\text{CO}_3)_3) + \\ & M(\text{Am}(\text{OH})_3) \\ & = 6.21811\text{E-}06 + 3.56989\text{E-}06 + 1.81972\text{E-}07 + 1.87358\text{E-}08 + 1.11489\text{E-}08 + 8.04118\text{E-}11 + 6.25941\text{E-}11 \\ & + 3.02061\text{E-}13 \\ & = 1.00000\text{E-}05 \end{aligned}$$

The input value for the elemental abundance total moles of Am is 1.00000E-05

Mass Balance for Thorium

Total moles of elemental thorium =

$$\begin{aligned} & M(\text{Th}(\text{CO}_3)) + M(\text{Th}(\text{OH})_3(\text{CO}_3)) + M(\text{Th}(\text{OH})_4) + M(\text{Th}(\text{SO}_4)_3) + M(\text{Th}(\text{SO}_4)_2) + M(\text{Th}) \\ & = 9.98187\text{E-}06 + 1.76010\text{E-}08 + 4.60620\text{E-}10 + 6.16159\text{E-}11 + 4.12197\text{E-}12 + 6.50005\text{E-}15 \\ & = 1.00000\text{E-}05 \end{aligned}$$

The input value for the elemental abundance total moles of Th is 1.00000E-05

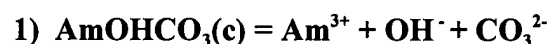
Mass Balance for Neptunium

Total moles of elemental neptunium =

$$\begin{aligned} & M(\text{NpO}_2) + M(\text{NpO}_2\text{CO}_3) + M(\text{NpO}_2\text{OH}) + M(\text{NpO}_2(\text{CO}_3)_2) + M(\text{NpO}_2(\text{CO}_3)_3) + M(\text{NpO}_2(\text{OH})_2) + \\ & M(\text{NpO}_2\text{CO}_3) \\ & = 6.00263\text{E-}06 + 1.36971\text{E-}07 + 1.00437\text{E-}09 + 1.95611\text{E-}10 + 3.33920\text{E-}12 + 1.01641\text{E-}14 + 3.85920\text{E-}06 \\ & = 1.00000\text{E-}05 \end{aligned}$$

The input value for the elemental abundance total moles of Np is 1.00000E-05

Reaction Equilibrium Calculations



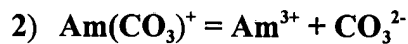
$$\frac{a(\text{Am}^{3+}) * a(\text{OH}^-) * a(\text{CO}_3^{2-})}{a(\text{AmOHCO}_3)} = \text{EXP}(\mu(\text{AmOHCO}_3) - \mu(\text{Am}^{3+}) - \mu(\text{OH}^-) - \mu(\text{CO}_3^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(1.14190E-07) * (2.55597E-08) * (9.81505E-09)}{(1.00000E+00)} = 2.86468E-23$$

For the right hand side (RHS) of the equation

$$EXP(-569.9800 - (-241.6940) - (-63.4350) - (-212.9440)) = EXP(-51.9070) = 2.86468E-23$$



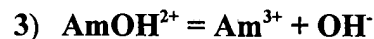
$$\frac{a(Am^{3+}) * a(CO_3^{2-})}{a(Am(CO_3)^+)} = EXP(\mu(Am(CO_3)^+) - \mu(Am)^{3+} - \mu(CO_3)^{2-})$$

For the left hand side (LHS) of the equation

$$\frac{(1.14190E-07) * (9.81505E-09)}{(4.12856E-08)} = 2.71470E-08$$

For the right hand side (RHS) of the equation

$$EXP(-472.060000 - (-241.6940) - (-212.9440)) = EXP(-17.4220) = 2.71470E-08$$



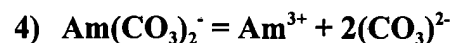
$$\frac{a(Am^{3+}) * a(OH^-)}{a(Am(OH)^{2+})} = EXP(\mu(Am(OH)^{2+}) - \mu(Am)^{3+} - \mu(OH)^{-})$$

For the left hand side (LHS) of the equation

$$\frac{(1.14190E-07) * (2.55597E-08)}{(8.03482E-11)} = 3.63252E-05$$

For the right hand side (RHS) of the equation

$$EXP(-315.35200 - (-241.6940) - (-63.4350)) = EXP(-10.22300) = 3.63252E-05$$



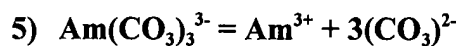
$$\frac{a(Am^{3+}) * (a(CO_3^{2-}))^2}{a(Am(CO_3)_2^-)} = EXP(\mu(Am(CO_3)_2^-) - \mu(Am)^{3+} - 2(\mu(CO_3)^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(1.14190E-07) * (9.81505E-09)^2}{(2.14327E-11)} = 5.13259E-13$$

For the right hand side (RHS) of the equation

$$EXP(-695.88000 - (-241.6940) - 2(-212.9440)) = EXP(-2.82980E + 01) = 5.13257E - 13$$



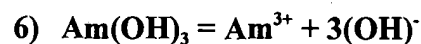
$$\frac{a(Am^{3+}) * (a(CO_3^{2-}))^3}{a(Am(CO_3)_3^{3-})} = EXP(\mu(Am(CO_3)_3^{3-}) - \mu(Am^{3+}) - 3(\mu(CO_3^{2-})))$$

For the left hand side (LHS) of the equation

$$\frac{(1.14190E-07) * (9.81505E-09)^3}{(1.60306E-16)} = 6.73528E-16$$

For the right hand side (RHS) of the equation

$$EXP(-915.46000 - (-241.6940) - 3(-212.9440)) = EXP(-3.49340E + 01) = 6.73529E - 16$$



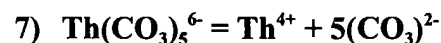
$$\frac{a(Am^{3+}) * a(OH^-)^3}{a(Am(OH)_3)} = EXP(\mu(Am(OH)_3) - \mu(Am^{3+}) - 3(\mu(OH^-)))$$

For the left hand side (LHS) of the equation

$$\frac{(1.14190E-07) * (2.55597E-08)^3}{(3.02061E-13)} = 6.31249E-18$$

For the right hand side (RHS) of the equation

$$EXP(-4.71603E + 02 - (-241.6940) - 3(-63.4350)) = EXP(-3.96040E + 01) = 6.31250E - 18$$



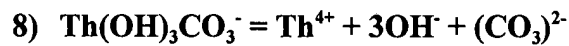
$$\frac{a(Th^{4+}) * (a(CO_3^{2-}))^5}{a(Th(CO_3)_5^{6-})} = EXP(\mu(Th(CO_3)_5^{6-}) - \mu(Th^{4+}) - 5(\mu(CO_3^{2-})))$$

For the left hand side (LHS) of the equation

$$\frac{(1.49019E - 16) * (9.81505E - 09)^5}{(1.76256E - 29)} = 7.70123E - 28$$

For the right hand side (RHS) of the equation

$$EXP(-1411.37800 - (-284.2270) - 5(-212.9440)) = EXP(-62.43100) = 7.70125E - 28$$



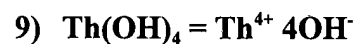
$$\frac{a(Th^{4+}) * a(OH)^3 * (a(CO_3^{2-}))^5}{a(Th(OH)_3(CO_3)^-)} = EXP(\mu(Th(OH)_3CO_3^-) - \mu(Th)^{4+} - 3(\mu(OH)^-) - (\mu(CO_3)^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(1.49019E - 16) * (2.55597E - 08)^3 * (9.81505E - 09)}{(4.69134E - 09)} = 5.20600E - 39$$

For the right hand side (RHS) of the equation

$$EXP(-775.62700 - (-284.2270) - 3(-63.4350) - (-212.9440)) = EXP(-8.81510E + 01) = 5.20604E - 39$$



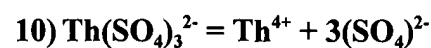
$$\frac{a(Th^{4+}) * a(OH)^4}{a(Th(OH)_4)} = EXP(\mu(Th(OH)_4) - \mu(Th)^{4+} - 4(\mu(OH)^-))$$

For the left hand side (LHS) of the equation

$$\frac{(1.49019E - 16) * (2.55597E - 08)^4}{(4.60620E - 10)} = 1.38077E - 37$$

For the right hand side (RHS) of the equation

$$EXP(-622.8400 - (-284.2270) - 4(-63.4350)) = EXP(-84.87300) = 1.38078E - 37$$



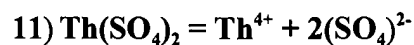
$$\frac{a(Th^{4+}) * (a(SO_4))^{3^2}}{a(Th(SO_4)_3^{2-})} = EXP(\mu(Th(SO_4)_3^{2-}) - \mu(Th)^{4+} - 3(\mu(SO_4)^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(1.49019E - 16) * (1.44317E - 03)^3}{(4.60620E - 10)} = 3.73819E - 13$$

For the right hand side (RHS) of the equation

$$EXP(-1214.00000 - (-284.22700) - 3(-300.38600)) = EXP(-28.61500) = 3.73821E - 13$$



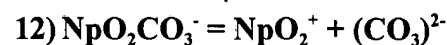
$$\frac{a(Th^{4+}) * (a(SO_4))^{2-}}{a(Th(SO_4)_2)} = EXP(\mu Th(SO_4)_2 - \mu (Th)^{4+} - 2(\mu (SO_4)^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(1.49019E - 16) * (1.44317E - 03)^2}{(1.21236E - 10)} = 2.56003E - 12$$

For the right hand side (RHS) of the equation

$$EXP(-911.69000 - (-284.22700) - 2(-300.38600)) = EXP(-26.69100) = 2.56004E - 12$$



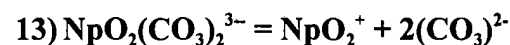
$$\frac{a(NpO_2^+) * (a(CO_3)^{2-})}{a(NpO_2(CO_3)^-)} = EXP(\mu NpO_2(CO_3)^- - \mu (NpO_2)^+ - (\mu (CO_3)^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(8.75343E - 06) * (9.81505E - 09)}{(9.20596E - 09)} = 9.33258E - 06$$

For the right hand side (RHS) of the equation

$$EXP(-593.63500 - (-369.10900) - (-212.94400)) = EXP(-11.58200) = 9.33257E - 06$$



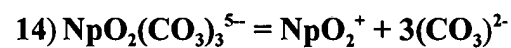
$$\frac{a(NpO_2^+) * (a(CO_3)^{2-})^2}{a(NpO_2(CO_3)_2^{3-})} = EXP(\mu NpO_2(CO_3)_2^{3-} - \mu (NpO_2)^+ - 2(\mu (CO_3)^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(8.75343E - 06) * (9.81505E - 09)^2}{(2.48933E - 15)} = 3.38751E - 07$$

For the right hand side (RHS) of the equation

$$EXP(-809.89500 - (-369.10900) - 2(-212.94400)) = EXP(-14.89800) = 3.38751E - 07$$



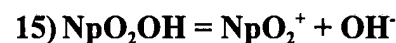
$$\frac{a(NpO_2^+) * (a(CO_3)^{2-})^3}{a(NpO_2(CO_3)_3^{5-})} = EXP(\mu NpO_2(CO_3)_3^{5-} - \mu (NpO_2)^+ - 3(\mu (CO_3)^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(8.75343E - 06) * (9.81505E - 09)^3}{(1.94047E - 24)} = 4.26529E - 06$$

For the right hand side (RHS) of the equation

$$EXP(-1020.30600 - (-369.10900) - 3(-212.94400)) = EXP(-12.36500) = 4.26529E - 06$$



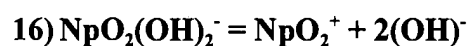
$$\frac{a(\text{NpO}_2^+) * a(\text{OH}^-)}{a(\text{NpO}_2\text{OH})} = \text{EXP}(\mu \text{NpO}_2(\text{OH})) - \mu (\text{NpO}_2)^+ - \mu (\text{OH}^-)$$

For the left hand side (LHS) of the equation

$$\frac{(8.75343\text{E} - 06) * (2.55597\text{E} - 08)}{(1.09586\text{E} - 10)} = 2.04164\text{E} - 03$$

For the right hand side (RHS) of the equation

$$\text{EXP}(-438.73800 - (-369.10900) - (-63.4350)) = \text{EXP}(-6.19400) = 2.04164\text{E} - 03$$



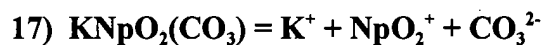
$$\frac{a(\text{NpO}_2^+) * a((\text{OH})^-)^2}{a(\text{NpO}_2(\text{OH})_2^-)} = \text{EXP}(\mu \text{NpO}_2(\text{OH})_2^-) - \mu (\text{NpO}_2)^+ - 2(\mu (\text{OH})^-)$$

For the left hand side (LHS) of the equation

$$\frac{(8.75343\text{E} - 06) * (2.55597\text{E} - 08)^2}{(1.65004\text{E} - 16)} = 3.46573\text{E} - 05$$

For the right hand side (RHS) of the equation

$$\text{EXP}(-506.24900 - (-369.10900) - 2(-63.4350)) = \text{EXP}(-10.27000) = 3.46574\text{E} - 05$$



$$\frac{a(\text{K}^+) + a(\text{NpO}_2^+) * a((\text{CO}_3)^{2-})}{a(\text{NpO}_2(\text{CO}_3))} = \text{EXP}(\mu \text{NpO}_2(\text{CO}_3) - \mu(\text{K}^+) - \mu(\text{NpO}_2^+) - 2(\mu(\text{CO}_3)^{2-}))$$

For the left hand side (LHS) of the equation

$$\frac{(2.90955\text{E} - 01) * (8.75343\text{E} - 06) * (9.81505\text{E} - 09)}{(1.00000\text{E} + 00)} = 2.49975\text{E} - 14$$

For the right hand side (RHS) of the equation

$$\text{EXP}(-727.33000 - (-113.95700) - (-369.10900) - (-212.94400)) = \text{EXP}(-3.13200\text{E} + 01) = 2.49975\text{E} - 14$$

It has been shown that mass balance and equilibrium constraints on Am(III), Th(IV), and Np(V) have been satisfied. Therefore, the acceptance criteria is considered to have been met.

7.0 RELATED TESTING DOCUMENTATION

Table 7.0.1 Documentation Related to the Testing of FMT
 (Page 1 of 2)

Test Item	Description	SCMS Filename
FLINT Output	Output generated as a result of running the source code analyzer, FORTRAN-Lint	FMT_QB0204.FLI
Scripts used and Log Files	Command files used to run the PCA analysis and test cases and the resulting log files	FMT_PCA_QB0204.COM FMT_PCA_QB0204.LOG FMT_TEST_QB0204.COM FMT_TEST_QB0204.LOG
SCA Output	Output generated as a result of running the source code analyzer, DECset-SCA	FMT_SCA_MOD_NOT_REF_QB0204.TXT FMT_CALLTREE_QB0204.TXT FMT_MODULES_QB0204.OUT
PCA Output	Output generated as a result of running the program coverage analyzer, DECset-PCA	FMT_COVER_CUM_QB0204.TXT
Input Files	Input files required to perform both the PCA analysis, and the functional testing.	FMT_SPC_BM.IN FMT_SPC_BM.INGUESS FMT_NP_NACL_BM.IN FMT_NP_NACL_BM.INGUESS FMT_THO2_6MNAACL.IN FMT_THO2_6MNAACL.INGUESS FMT_AM_NA2CO3.IN FMT_AM_NA2CO3.INGUESS FMT_AM_NAHCO3.IN FMT_AM_NAHCO3.INGUESS FMT_AMPO4_SO4_BM1.IN FMT_AMPO4_SO4_BM1.INGUESS FMT_AMPO4_SO4_BM2.IN FMT_AMPO4_SO4_BM2.INGUESS FMT_FCO2_PH_FIXED.IN FMT_FCO2_PH_FIXED.INGUESS FMT_INVAR_M.IN FMT_INVAR_M.INGUESS FMT_INVAR_B3.IN FMT_INVAR_B3.INGUESS FMT_INVAR_K4.IN FMT_INVAR_K4.INGUESS FMT_AMTHNP_SPC.IN FMT_AMTHNP_SPC.INGUESS
Output Files from Testing Tools	Output files resulting from running the testing tools.	FMT_

Table 7.0.1 Documentation Related to the Testing of FMT
 (Page 2 of 2)

Test Item	Description	SCMS Filename
Output Files from Testing Tools	Output files resulting from running the testing tools.	FMT_SPC_BM_QB0204.OUT FMT_NP_NACL_BM_QB0204.OUT FMT_NP_NACL_BM_QB0204.TITRATE FMT_THO2_6MNAACL_QB0204.OUT FMT_THO2_6MNAACL_QB0204.TITRATE FMT_AM_NA2CO3_QB0204.OUT FMT_AM_NA2CO3_QB0204.TITRATE FMT_AM_NAHCO3_QB0204.OUT FMT_AM_NAHCO3_QB0204.TITRATE FMT_AMPO4_SO4_BM1_QB0204.OUT FMT_AMPO4_SO4_BM1_QB0204.TITRATE FMT_AMPO4_SO4_BM2_QB0204.OUT FMT_AMPO4_SO4_BM2_QB0204.TITRATE FMT_FCO2_PH_FIXED_QB0204.OUT FMT_INVAR_M_QB0204.OUT FMT_INVAR_B3_QB0204.OUT FMT_INVAR_K4_QB0204.OUT FMT_AMTHNP_SPC_QB0204.OUT

8.0 CONCLUSION

The testing for FMT as prescribed in the Verification and Validation Plan has been completed and all acceptance criteria have been satisfied. The set of test cases provided in Section 6 provide complete coverage of all functional requirements as described in Section 6.0.

9.0 REFERENCES

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- WIPP-PA - Requirements Document/Verification and Validation Plan for FMT Version 2.40 WPO# 51305
- 4) WIPP-PA - User's Manual for FMT Version 2.30, WPO# 43037

10.0 APPENDICES

APPENDIX A: REVIEWER'S COMMENTS

(See attached sheets)

Information Only